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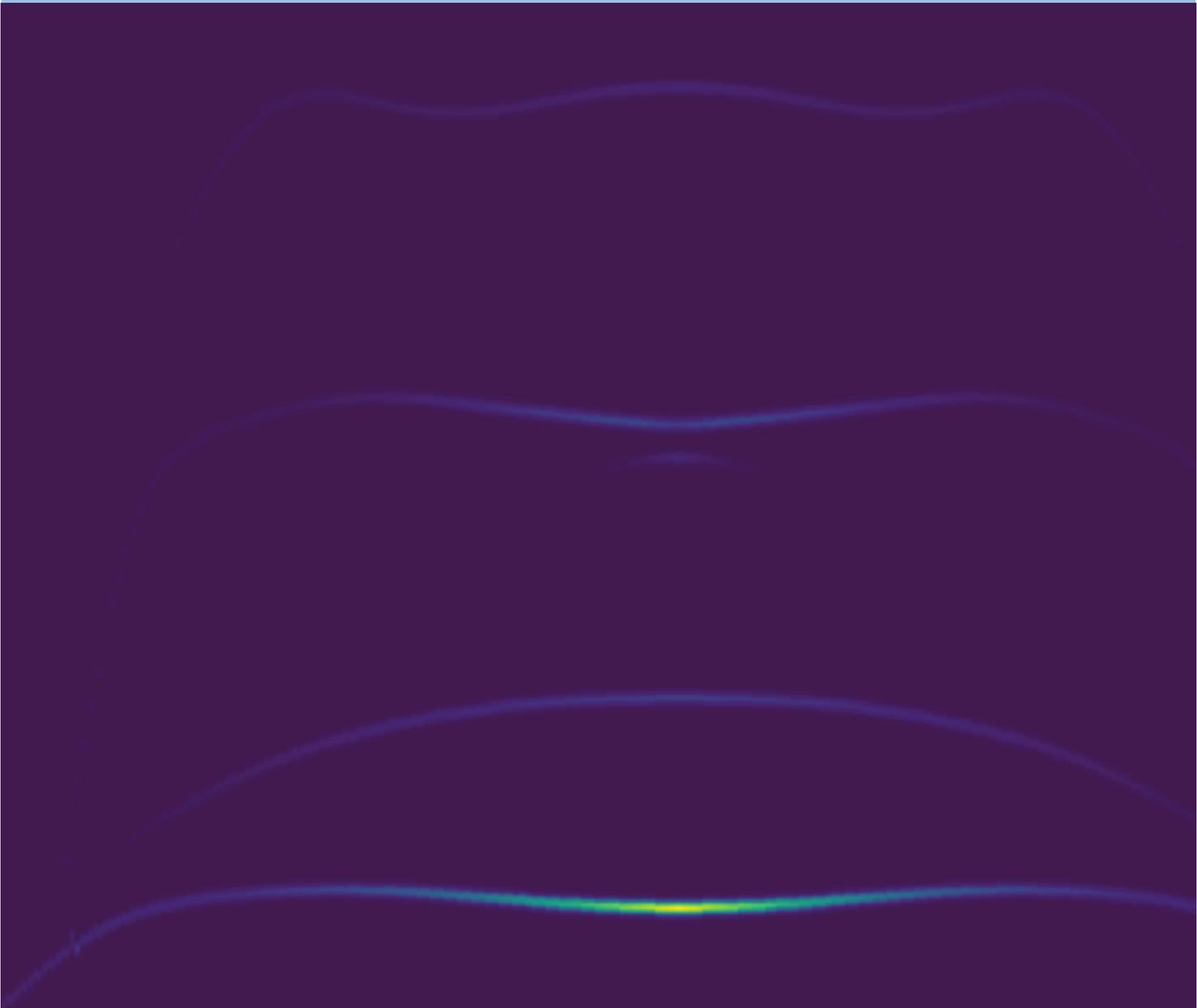
DEPARTMENT OF MATHEMATICS AND PHYSICS

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# **Harmonic Phonon transport in Strontium Titanate: experiment vs computation**

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Master's Thesis - - June 2023



I, **Shibl Gill**, declare that this thesis titled, “Harmonic Phonon transport in Strontium Titanate: experiment vs computation ” and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a master’s degree at the University of Stavanger.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.

*“The creation of Physics is the shared heritage of all mankind. East and West, North and South have equally participated in it. ”*

– Abdus Salam

# Abstract

Thermoelectric materials can be a boon for the temperature regulation industry, however, before its popular use as a green energy management solution, it is imperative that we uncover thermal transport in these materials. In the effort to discover better suited thermoelectrics, it is imperative that we are able to develop and test *ab initio* computational modelling methods to gain insight into the electronic and thermal properties of materials. This is not only cheaper and easier than neutron scattering experiments, but may also allow us to discover new materials that have the desired transport properties.

In this thesis, we examine how well Density Functional Theory (and its derivatives) are able to model electronic and phonon properties in a well known pyroovskite thermoelectric, strontium titanate (STO). We used a number of DFT calculational software to probe the electronic and phonon dispersions, densities of state and dynamic structure factor of STO, and compare those results to inelastic neutron scattering results from the CAMEA multiplexing spectrometer at the Paul Schreer Institute in Switzerland.

Another aspect of materials physics presented in this thesis is that of science communication and outreach in the form of the "Shaking Matters" podcast produced and hosted by myself.

# Acknowledgements

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My thanks also go to my university, Universitetet i Stavanger where I have found an invigorating environment for scientific curiosity and inquiry, and to the NETTOP department for their help with the Shaking Matters podcast project. Thanks also goes to my classmate Zaryab Khatri, and postdoc Quoc Duy Ho for their support. The podcast was funded by the PHUN project (number 324863) at the Norwegian Research council, and I should like to thank the benefactors and all the guests that took the time to be interviewed, including SINTEF researchers Dr. Frittita, Dr. Sagvolden, Joanna Lewis at the ESS, Dr. Nemkovsky and his colleagues at ISIS, and Dr. Toft-Ptereson at the Danish Technical University.

I should also like to acknowledge the love and support of my family, and my partner Live Skeie whose fastidious support throughout this year has been invaluable and heart-touching.

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# Chapter 1

## Introduction to the Thesis

The work carried out in this thesis is primarily concerned with computationally calculating the harmonic approximation of phonons in Strontium Titanate, and comparing the results with inelastic neutron scattering experimental data. Computational methods and results are explained in detail, along with details about the experimental setup and its findings.

### 1.1 Thermoelectric Materials

In this chapter we discuss the basic theory of thermoelectric materials, thermoelectric phenomena such as the Seebeck and Peltier effects, and the relevant mathematical formulations.

Converting heat directly into electricity efficiently, or vice versa, can be the panacea our modern world needs as we stumble knowingly into a crisis of energy and our ecology. It is evident, however, that a singular solution cannot intervene in the large-scale climatic change processes currently at work, but a brighter future can only be attained by tapping into all available scientific recourses available to us. In this effort, thermoelectric materials can prove to be a saving grace, if we are able to tackle the central challenges that currently stifle the growth of the field: efficiency of energy conversion. Success in tackling this problem will inevitable lead to viable alternatives to traditional means of temperature regulation. The

International Energy Agency (IEA) reports that 50% of global final energy consumption is used for heating and this accounts for 40% of global carbon dioxide emissions. Energy use for cooling is also significant and has a similar emission profile, with the added drawback of environmental pollution caused by refrigeration gases [1].

In the early 19<sup>th</sup> century, thermoelectric effects became known to the scientific community through the works of Seebeck in 1821, and Peltier in 1834. Two sides of the same proverbial coin, these effects form the cornerstone of inquiry into thermoelectrics. Let's take a closer look at each of them:

### **The Seebeck Effect**

Seebeck discovered that given an electrically conductive material with a temperature gradient between two points  $\nabla T$ , an electromotive force  $E_{emf}$  is produced between the two points:

$$\sigma_s = \frac{E_{emf}}{\nabla T}$$

with  $\sigma_s$  being the Seebeck coefficient. This works on the principles that free charge carriers can also transport thermal energy. When a thermoelectric material experiences a temperature gradient, charge carriers migrate down the gradient, inducing a measurable voltage across the two points [2].

### **The Peltier Effect**

Thirteen years after Seebeck's discovery, Jean Peltier uncovered the analogous Peltier effect whereby a temperature gradient is observed when a voltage is applied between two conductors. Later, it was Lenz who noted that the effect seen in different metals was a consequence of the direction of current flow. The Peltier coefficient  $\pi_p$  is therefore similarly defined as:

$$\pi_p = \frac{P}{I}$$

With  $P$  denoting the power generated at the junction of the two metals, and  $I$  the current applied.

When the famed Lord Kelvin was looking into these peculiar effects, he came up with a simple yet effective insight: these two constants can be related as

$$\pi_p = \sigma_s * T$$

### **1.1.1 The Thermoelectric Figure of Merit**

The thermoelectric figure of merit  $\zeta$  is a dimensionless quantity that is a measure of a thermoelectric system in converting thermal energy into electrical energy, or vice versa. A higher figure of merit corresponds to a higher proportion of energy conversion. It is defined as:

$$\zeta T = \frac{\sigma_s^2 \alpha}{\kappa} T \tag{1.1}$$

Where  $\alpha$  and  $\kappa$  are electrical and thermal conductivity [2].

## **1.2 The Shaking Matters Podcast**

During the year spent on this thesis, I produced a materials science podcast titled "Shaking Matters" with the byline "Materials Science and Sustainability with Shibl Gill". Working under guidance from my thesis advisor Dr. Diana Lucia Quintro Castro, I researched, hosted and produced three full episodes at the time of the submission of this thesis. The podcast is intended to bring materials science to a wider audience by featuring interviews with researchers, instrumentalists, science policy makers and science communicators.

This podcast was proposed in the program outline of the PHUN (Phonon lifetimes; unifying inelastic neutron scattering measurements with first-principle calculations) project funded by the Norwegian Research Council, where Dr. Diana Lucia is the project manager.



Figure 1.1: Shaking Matters podcast cover art

The podcast cover art produced with the help of the UiS NETTOP department is shown in Fig.1.1.

The interviews and discussions held in the podcast episodes helped me to gain a broader understanding of the theory behind, and the techniques used in this thesis. In the first episode, I discussed *ab initio* methods with Dr. Espen Sagvolden and Dr. Edoardo Fertitta at SINTEF.

For the second episode, I visited the ISIS Neutron and Muon source at the Rutherford Appleton research lab in the UK. Here, I spoke with Dr. Kirill Nemkovskiy and other instrument and computational scientists about neutron instrumentation and developments in the field. I also spoke with students interning at the lab about their motivations and experiences.

The third episode was recorded at the European Conference for Neutron Scattering (2023) at Garching, Germany. I was joined by Joanna

Lewis, a science outreach coordinator from the European Spallation source (ESS) and Dr. Rasmus Toft-Peterson, affiliated with the Danish Technical University and working on the BIFROST instrument under development at the ESS.

Science communication, and in particular, informal science communication is a topic that greatly interests me and therefore I volunteered to take the project on. Transcripts of the interviews conducted so far are given in the Appendix.

# Chapter 2

## Background Theory

In this chapter we begin with a short introduction to quantum mechanics to the extent that is required to fully appreciate this thesis. We will go through the basic building blocks of Density Functional Theory (DFT), exchange and correlational functionals, some commonly used examples of the same, and we will also discuss the fundamental theory of phonons. Armed with this background, we will be able to analyse the methods used, and the results produced later on.

### 2.1 Quantum Mechanics Basics

In this chapter we will briefly look at the theoretical foundations upon which the work done in this thesis rests. We will start with the very basics of quantum physics, how dynamics can be defined and analysed in the quantum realm.

The most successful basic theory for uncovering system dynamics for a quantum system is the quantum mechanical wave equation, the Schrödinger equation. This differential equation describes how a wavefunction  $\psi$  evolves under a potential  $V(r)$ . For a non-relativistic system with a three dimensional potential  $V(r)$ , we have:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \hat{H}\Psi(\mathbf{r},t) \quad (2.1)$$

Where  $\hat{H}$  of course is the Hamiltonian operator, a sum of the kinetic energy operator and the external potential. In the quantum regime, any physical observable is associated with a self-adjoint linear operator. Now for a particle of mass  $m$ , the Hamiltonian has the well-known form:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \quad (2.2)$$

### 2.1.1 Operators

A linear operator is of the form:

$$\Omega(af) = a\Omega f \quad (2.3)$$

A fundamental postulate of quantum mechanics states that all possible result of a quantum measurement represented by some operator  $\Omega$  are its eigenvalues  $\Omega_i$ :

$$\Omega\Psi_i = \Omega_i\Psi_i \quad (2.4)$$

And for the time independent Schrödinger equation, the eigenvalue of the Hamiltonian operator is the total energy of the system [3].

$$\hat{H}\Psi = E\Psi \quad (2.5)$$

### 2.1.2 Electronic Structure

It is known that in quantum mechanics, the entire state of a system can be described by its wavefunction which depends on the spin and spatial coordinates of all particles in the system.

$$\Psi_n(x_1, x_2, \dots, R_1, R_2, \dots, R_m) \quad (2.6)$$

Wavefunctions are solutions to the molecular Schrödinger equation (2.1). If the wavefunction  $\Psi_n$  is known, then we obtain any time-independent observable by computing the expectation value:

$$\int \Psi_n^*(\tau) \hat{\Omega} \Psi_n(\tau) d\tau \quad (2.7)$$

## 2.2 The Quantum Many Body Problem

As we know, solids consist of many heavy positively charged nuclei and relatively much lighter negatively charged electrons. So for  $n$  nuclei, we have to tackle a problem with  $n + Zn$  electromagnetically interacting particles. Now the Schrödinger equation we have considered so far only has exact solutions for simple cases such as the hydrogen atom, or the well-known particle in a box. It is not possible to analytically solve the Schrödinger equation for an enormous number of particles and their interactions even with the help of the most capable computers.

Additionally, to solve the Schrödinger equation analytically, we need a suitable basis and Hamiltonian operator. For large systems, we require efficient and accurate bases and Hamiltonians, which is again a tall order for such systems [3].

The exact form of a many-body Hamiltonian is given as follows:

$$\hat{H} = -\frac{\hbar^2}{2} \sum_i \frac{\nabla_{\mathbf{R}_i}^2}{M_i} - \frac{\hbar^2}{2} \sum_i \frac{\nabla_{\mathbf{r}_i}^2}{m_e} - \frac{1}{4\pi\epsilon_0} \sum_{i,j} \frac{e^2 Z_i}{|\mathbf{R}_i - \mathbf{r}_j|} + \frac{1}{8\pi\epsilon_0} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{8\pi\epsilon_0} \sum_{i \neq j} \frac{e^2 Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} \quad (2.8)$$

[2]

We have terms representing (in order of appearance):

- Kinetic energy of ions
- Potential energy of ions
- Kinetic energy of electrons
- Electron-electron interactions
- Electron-ion interactions

### 2.2.1 The Born-Oppenheimer Approximation

Since nuclei are much more massive than electrons, their dynamics will be much slower than electrons' and therefore we can start our approximation journey with the Born-Oppenheimer Approximation. It assumes the nuclei are frozen in their positions, and the electrons are in an instantaneous equilibrium around them. The nuclei, then, are relegated to the status of simply being the sources of positive potential, external to the electron cloud. We then have a collection of negatively charged mobile particles moving in an external positive potential.

How does this first simplification affect the Hamiltonian (2.8)? The nuclear kinetic energy is zero and Columbic interaction between nuclei is reduced to a constant. What remains is the kinetic energy of the electrons, their potential energy due to nuclear potential and electron-electron interactions. We can write this as:

$$\hat{H} = \hat{T} + \hat{V} + \hat{V}_{\text{ext}} \quad (2.9)$$

And we are interested in finding the eigenstates of the stationary Schrödinger equation:

$$\hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle \quad (2.10)$$

However, because we still have the electron-electron interaction term, the equation is not separable. This foreshadows that we need to further refine our approximations if we are to find a viable solution.

### 2.2.2 Hartee-Fock Self Consistency Method

In this next rung on the ladder of trying to analytically solve the many-body Schrödinger equation, we begin by approximating the wavefunction of the many-body system as a product of single electron wavefunctions: the total Hamiltonian is the sum of single electron Hamiltonian operators

$H_i$ . We formulate the single electron wavefunctions as spin orbitals:

$$\Psi(r_1, r_2, \dots, r_n) = \chi_1(r_1)\chi_2(r_2)\dots\chi_n(r_n) \quad (2.11)$$

This form of the wavefunction is known as the Hartree product and each spin orbital is a product of a function and one of two available spin states [4]. However, this formulation fails to satisfy the many electron wavefunction prerequisite of the Antisymmetry Principle. Therefore we revert to the known Slater Determinate formulation and arrive at Hartree Fock Theory.

The Slater Determinant has the form:

$$\begin{array}{cccc} \psi_1(\mathbf{r}_1, \sigma_1) & \psi_2(\mathbf{r}_1, \sigma_1) & \cdots & \psi_{2N}(\mathbf{r}_1, \sigma_1) \\ \psi_1(\mathbf{r}_2, \sigma_2) & \psi_2(\mathbf{r}_2, \sigma_2) & \cdots & \psi_{2N}(\mathbf{r}_2, \sigma_2) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_1(\mathbf{r}_N, \sigma_N) & \psi_2(\mathbf{r}_N, \sigma_N) & \cdots & \psi_{2N}(\mathbf{r}_N, \sigma_N) \end{array} \quad [3]$$

Hartree Fock Theory is discussed in detail in many textbooks, and works well for atoms and molecules, hence often used in quantum chemistry. Here, however, since we are interested in crystalline solids, we move on to the main approximation used in this thesis, Density Functional Theory.

## 2.3 Density Functional Theory

The basic idea behind implementing DFT is to reduce the parameter space. Due to its computational accuracy, DFT is the most popular method for computationally working out electronic structure.

The first step in our DFT journey will be to write the energy of the system as a function of the electron probability density  $\rho(r)$ , this was first proposed by, and is built upon the proof by Hohnberg and Kohn [5]. They showed that the ground state electronic energy is built completely out of the electron density functional  $E(\rho)$ .

### 2.3.1 Computational considerations of DFT

Consider the wavefunction of a system of  $n$  electrons. This wavefunction then contains  $3n$  coordinates, three spatial coordinates for each electron; upon which depends the electron density. Of course, the complexity of DFT calculations is directly correlated with the number of electrons in the system, but we have the advantage of working in a three dimensional parameter space. We use a single three dimensional function to describe the dynamic of an  $n$  electron system, whereas to describe the same dynamics using the wavefunction approach, we would require a minimum of a  $3n$  dimensional function with constraints ensuring full antisymmetry.

### 2.3.2 Hohenberg-Kohn Theorems

The following two theorems form the pillars upon which the validity of the Density Functional Theory methodology rests. These theorems apply to any system of electrons in an external potential. [5]

**Theorem I: The external potential  $V(\vec{r})$  is (except for an additive constant) uniquely determined by the electron density  $\rho(\vec{r})$ .** Alternatively: **There are no two different  $V(\vec{r})$ ,  $V'(\vec{r})$  that have the same electron density  $\rho(\vec{r})$ .**

The ground-state  $\rho(\vec{r})$  uniquely determines the potential and thus all ground state properties.

**Theorem II: the ground state energy of a many electron system can be expressed as a unique functional of electron density  $\rho(\vec{r})$**

Now since the ground state depends on  $\rho(\vec{r})$ , we can define the energy functional as:

$$E[\rho(\vec{r})] = F[\rho(\vec{r})] + V_{\text{ext}}[\rho(\vec{r})] \quad (2.12)$$

Here,  $F$  is the internal energy, and  $V_{\text{ext}}[\rho(\vec{r})]$  are the external potential energy functionals of the electron density.

These theorems allow us to write the Hohnberg-Kohn energy as:

$$E[\rho(\vec{r})] = T[\rho] + V_{ee}[\rho] + \int \rho(\mathbf{r})v_{ext}(\mathbf{r})d\mathbf{r} \quad (2.13)$$

with

$$F[\rho(\vec{r})] = T[\rho] + J[\rho] + E_{xc}[\rho] \quad (2.14)$$

Where  $T[\rho]$  is the kinetic energy,  $J[\rho]$  is the Columbic electron interaction energies, and

$$E_{xc}[\rho] = E_x[\rho] + E_c[\rho] \quad (2.15)$$

are the exchange and correlation energies respectively.

As it happens, the exact functional that relates total energy and electron density is not known. In fact, we need to obtain somehow the functionals that define the Kinetic, exchange and correlational energies.

### 2.3.3 Kohn-Sham Theory

The Kohn-Sham equations provide a mechanism to arrive at the exact ground-state density, and thereby also the corresponding energy. In this formalism we split the kinetic energy functional into two: one part that can be calculated exactly and a correction term. As for the electrons, the potential they feel is due to the nuclei is dependent on particle density, but the other terms only depend on density implicitly.

Starting with basing our unknown functionals on products of an antisymmetrised spin-orbitals, the approximate density is given as a set of one-electron spin orbitals:

$$\rho(r) = \sum_{i=1}^N |\phi_i(r)|^2 \quad (2.16)$$

for  $N$  electrons. Here we restrict the range of densities. Then by requiring orthogonal orbitals and minimising the functional with Lagrange multi-

pliers, we can arrive at the Kohn-Sham equations:

$$\hat{H}_{\text{KS}}\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r}) \quad (2.17)$$

and to calculate the density of non-interacting particles:

$$\left[\frac{1}{2}\nabla^2 + v_{\text{eff}}(\mathbf{r})\right]\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r}) \quad (2.18)$$

The challenge now is not to locate the all-encompassing H-K functional, but rather to identify the hypothetical arrangement of non-interacting electrons that exhibit identical density to that of the true system containing interacting electrons [6].

So, starting with constructing and solving the Schrödinger equation for one electron, we combine many one-electron wavefunctions to produce an approximate wavefunction for all electrons. Then, the density of a 'fictitious' system non-interacting electrons gives us the exact density of interacting electrons, the molecular orbitals. Then we build the density  $n_0(r)$  from the molecular orbitals to compute the energy  $E[n_0]$

### 2.3.4 Local Density Approximation

In theory there exists an exchange and correlational functional  $E_{XC}[n(r)]$  that contain all inter-electron Coloumbic interaction energy information, but that functional is unknown. Therefore we need to approximate this functional by analysing systems that are patently describable. If we consider an enclosed space filled with a uniform gas and set the electron density  $n[r]$  to be constant throughout space, then the Local Density Approximation (LDA) is a suitable  $E_{XC}$ . It was introduced by Kohn-Sham in their original 1965 paper outlining KS theory [6].

$$E_{xc}^{\text{LDA}} = \int \epsilon(n(\mathbf{r}))n(\mathbf{r})d\mathbf{r} \quad (2.19)$$

Here, the  $\epsilon$  is a parameter attributed to the exchange and correlation in a uniform electron gas and can be numerically calculated. The LDA has

proved to be a successful approximation for most materials. If we were to further refine our approximation and consider the exchange and correlation of a uniform electron gas with its gradient, we arrive at the next level of XC approximation: the Graduated Gradient Approximation (GGA). This functional also accounts for the local gradient of  $n(r)$ . However, it is known that this functional is computationally more bulky, and results from comparison with LDA are mixed. This is why modified GGA functionals that are tailored for certain materials or calculations are often used. The PBE-GGA functional -named after Perdew, Becke and Ernzerhof (1996) [7]- is one of the most common GGA based functionals used. PBE-GGA is one of the most commonly used functionals in this thesis.

### **The Modified-Becke-Johnson functional (mBJ)**

WIEN2k has the builtin capability to choose from a few different XC functionals and the mBJ was identified as one such promising functional for STO. This functional has been proven to provide a more accurate estimation of band gaps, without being computationally overly expensive [8]. Later in the Results chapter, we shall compare the electronic band structure of STO using standard PBE-GGA and mBJ potentials.

## **2.4 Phonons and their Properties**

Phonons are pseudo-particles that can be described as a quanta of mechanical energy in a material. Phonon properties in a material partly determine its thermal properties. Phonons occur primarily in either acoustic (coherent collective motion of atoms from their equilibrium positions), or optical (out of phase motion of atoms) modes [2].

### **2.4.1 Waves in a lattice- Harmonic Approximation**

There are three types of thermal energy transfer mechanisms: conduction, convection and radiation. Heat transfer in crystalline condensed matter

systems is characterised by lattice vibrations of atoms around their equilibrium positions, with a linear restoring force: this is modeled by the classical harmonic approximation.

Since we are describing the energy of a lattice that can be approximated by a series of harmonic oscillators, we term this the harmonic approximation. This is a mathematically convenient approximation as harmonic equations of motion have exact solutions, and provide a realistic picture of a system at low temperature. This is still a worthwhile avenue of inquiry for a number of reasons:

1. At low temperatures, the harmonic term is the only substantial contribution to lattice dynamics - since amplitudes of displacement are lower
2. The harmonic approximation allows us to capture physical properties of the system reasonably well
3. Beginning with the simplest model, as is the general practice in physics, we can always add perturbations to the theory in order to correct the simplest model to map more complex dynamics.

Within a crystalline lattice, we begin by defining the dynamics of atomic displacements from their equilibrium positions. Assuming the inter-atomic forces to be approximated by the spring constant  $\gamma$ , and lattice constant  $a$ , the equation of motion for some atom  $n$  with mass  $M$  can be given as:

$$M \frac{d^2 u_n}{dt^2} = -\gamma(u_n - u_{n-1}) + \gamma(u_{n+1} - u_n) \quad (2.20)$$

[9]

A wave defined at the lattice sites solves this equation

$$u_n(t) = u e^{i(kan - \omega t)} \quad (2.21)$$

With  $k = 2\pi/\lambda$  is the wave vector and  $u$  the amplitude. Using this solution

for 2.20, we get:

$$\omega(k) = \sqrt{\frac{2\gamma(1 - \cos(ka))}{M}} \quad (2.22)$$

Such a relationship connecting the frequency to the wavevector is termed the dispersion relation. And one particular solution with  $\omega(k)$  is a normal mode of vibration. To describe heat transport by lattice vibrations, it is important to consider the boundary conditions which will prescribe the treatment of the termini of a lattice structure. Here, we consider the Born-Karman boundary conditions [10] proposed in 1912:

$$u_{N+n}(t) = u_n(t) \quad (2.23)$$

Also known as the cyclic boundary condition as we consider a chain of atoms that where the end is affixed to the beginning. This allows us to consider an infinite crystal lattice whilst describing the properties of a finite crystal.

Now a set of discrete allowed values of  $K$  of the below form emerge:

$$k = \frac{2\pi}{aN}m \quad (2.24)$$

$m$  is any integer from 0 to  $N$  and we can see that vibrations remain unaffected upon the addition of reciprocal lattice vectors:  $\frac{2\pi}{a}$ . Each  $k$  represents a phonon wavevector, and we can choose certain values of  $k$  that lie within the Brillouin zone. In fact, the range of wavevectors in reciprocal space gives us the first Brillouin zone:  $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$ .

So far, we have considered the wave-like character of phonons, however, in order to consider thermal transport properties, it is important to consider their "particle-like" character. In the quantum mechanical treatment, then, normal modes can be excited in discrete energy quanta multiples of  $\hbar$  and  $\omega(k)$ .

### 2.4.2 Generalising to 3-dimensions

Since any atom in a periodic crystal lattice is inextricably linked to other atoms in the structure, we must consider the dynamics of the entire system as a single entity. But we can exploit the basic fact that the periodic arrangement of atoms means that in three dimensions, we decompose the wavevector  $k$  to its three components [9]. Then for  $N$  atoms with lattice spacing  $a$  we get:

$$\mathbf{k} = \frac{2\pi}{aN}(n_x, n_y, n_z) = \left( \frac{2\pi}{L}n_x, \frac{2\pi}{L}n_y, \frac{2\pi}{L}n_z \right) \quad (2.25)$$

with  $n_i$  being integers, and  $L$  the macroscopic length of the crystal.

It is again sufficient to describe vibrational states within the first Brillouin Zone: the first Brillouin Zone being the set of points closer to the reciprocal lattice point than to any other. The first Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice.

For our enquiry into the interactions between atoms in a periodic arrangement, we start with working out the force constants that govern the strength of crystalline dynamics. We can write the total energy of a lattice of  $n$  atoms at positions  $r_i$ , and displacements of the  $i$ -th atom from equilibrium as  $u_i$  as:

$$E = \frac{1}{2} \sum_{i,j} \Phi_{ij} u_i u_j \quad (2.26)$$

Now  $\Phi_{ij}$  represents the force constants. Then

$$F_i = -\frac{\partial E}{\partial u_i} = -\sum_j \Phi_{ij} u_j \quad (2.27)$$

With  $F_i$  is the force experienced by atom  $i$ . Rearranging gives us the below expression:

$$\Phi_{ij} = -\frac{\partial^2 E}{\partial u_i \partial u_j} \quad (2.28)$$

We Taylor expand the energy around the equilibrium positions to get:

$$E = E_0 + \sum_i \frac{\partial E}{\partial u_i} u_i + \frac{1}{2} \sum_{i,j} \frac{\partial^2 E}{\partial u_i \partial u_j} u_i u_j + \dots \quad (2.29)$$

Here,  $E_0$  is the energy at equilibrium positions, the second term is 0 since we defined the equilibrium positions by setting the force constants to 0, and the third expression gives us the force constants:

$$\Phi_{ij} = \frac{\partial^2 E}{\partial u_i \partial u_j} \quad (2.30)$$

Now, for a harmonic approximation, we are only interested in the force constant Taylor series up to the second derivatives, and the Hamiltonian is solvable. Then given the Born Von Karman periodic boundary condition and substituting a plane wave ansatz [2] of the form:

$$U_n = \sum_k \tilde{U}_k \exp(i[kna - \omega_k t]) \quad (2.31)$$

Here,  $k$  is the wavevector,  $\omega_k$  the angular frequency of a mode of oscillation, and  $\tilde{U}_k$  its amplitude.

This ansatz when substituted into the force constants expression will give us an eigenvalue equation that can describe the dynamical matrix  $D_{\alpha\beta}$ . I will not describe its derivation in detail here [11].

The dynamical matrix is hermitian for any values of  $q$  and contains  $3n \times 3n$  elements. So there are  $3n$  frequencies for any value of  $q$ .

The phonon dispersion relation is the relationship between phonon frequency and wavevector. Phonon dispersion is theoretically possible at all phonon modes, however, as we shall see, some phonon modes are unphysical.

### 2.4.3 Density Functional Perturbation Theory

As noted earlier, DFT and other *ab initio* methods are highly successful methodologies for describing structure and phenomena in crystallographic materials. Now, DFPT is a branch of DFT that considers how a system responds when a small perturbation is introduced; and as such, DFPT is especially suited to describing vibrational properties of a material -its phonon character. Starting with the familiar Kohn-Sham scheme, effective potentials and electron wavefunctions, the ground state energy is obtained and then solved using appropriate exchange and correlational functionals [12]. Then perturbations to the ground state energy configuration are introduced and the electron density is expanded in terms of perturbation strength. This allows us to obtain response functions that describe the perturbation in terms of ground state energy quantities. The response functions are derivatives of the energy with respect to the perturbations. Phonon properties are encapsulated in the second order derivatives.

We will be exploiting the DFPT capabilities built into Quantum Espresso later on to calculate phonon properties in strontium titanate.

# Chapter 3

## Methods

### 3.1 Computational Methods

Computational methods of modelling crystallographic systems have been used to probe material properties for decades now, and have proven to reproduce real-world phenomena to a very reasonable degree. These methods include DFT, Molecular Dynamics, and Monte Carlo simulations. For our purposes, DFT and its derivatives are most relevant.

#### 3.1.1 Benchmarking in WIEN2k with TiC

WIEN2k uses a linearised augmented plane wave method, along with local orbitals (APW+LO) [13]. Working on the Kohn-Sham scheme where the system in question is characterised by KS orbitals and a specific KS energy. One can then fill these KS orbitals as a function of their KS energies, leading us to the exact electron densities. Then we must of course address the requirements of an exchange correlational functional and the matching exchange correlational potential. WIEN2k considers a repeating periodic arrangement of unit cells corresponding to periodic boundary conditions.

In APW methods, WIEN2k employs a muffin-tin approach where the unit cell is decomposed into spheres centered at nuclear sites, and interstitial regions. This allows the DFT code to consider the full electron-nucleus potential and to explicitly handle both valence and core electrons.

I used WIEN2k version 19.2 in this thesis and further details and references can be found in the WIEN2k user guide [13].

### **3.1.2 Initialising a WIEN2k Calculation**

The International Tables of Crystallography is an invaluable resource that provides crystallographic and structural information on materials being considered. For TiC (and later STO) positions of equivalent atoms, the lattice type and lattice parameters were collected and passed to the "Struct-Gen" functionality in WIEN2k.

Then the appropriate input files are created by following a scheme of initialising steps that include the below:

1. nn: determines inter-atomic distances and thereby calculates atomic sphere radii
2. Sgroup: determines the spacegroup and smallest primitive cell
3. Symmetry: finds the symmetry operations of the spacegroup and the point group symmetry.
4. lstart: Solves the radial Dirac equation for free atoms and calculates atomic densities. The user then selects from available exchange and correlational potential, and energy at which valence and core states are separated.
5. kgen: User specifies the number of  $K$  points to be sampled in the Brillouin zone
6. dstart: based on lstart atomic densities, generates a starting density for the SCF cycle

Then we are prompted with the option to begin the Self Consistency Cycle. A schematic for this workflow is given below in Figs. 3.2 and 3.1 [14].

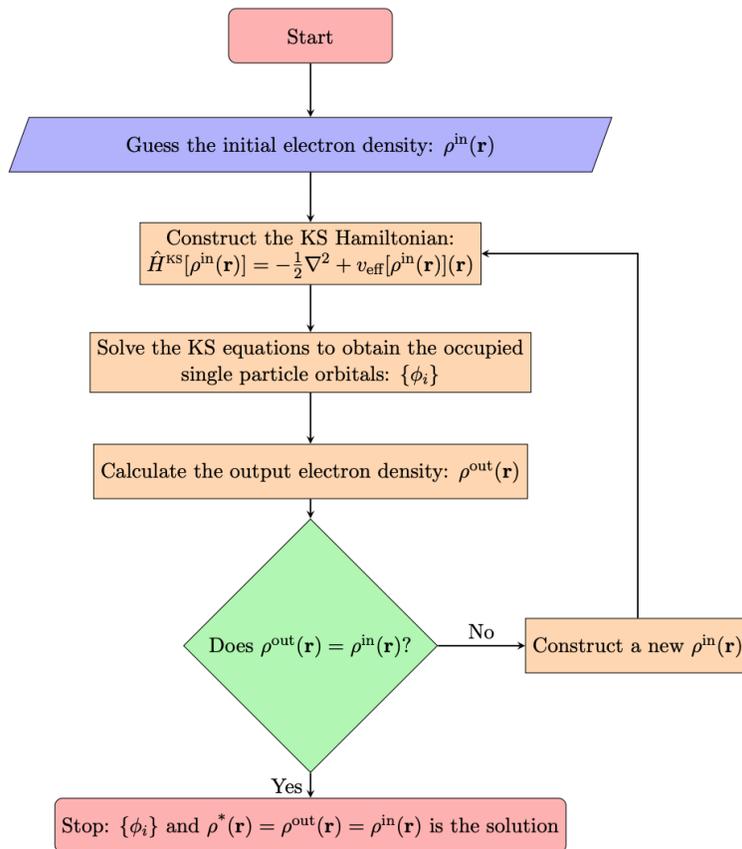


Figure 3.1: Flowchart showing the self consistent solution to the Kohn-Sham equations. From [14]

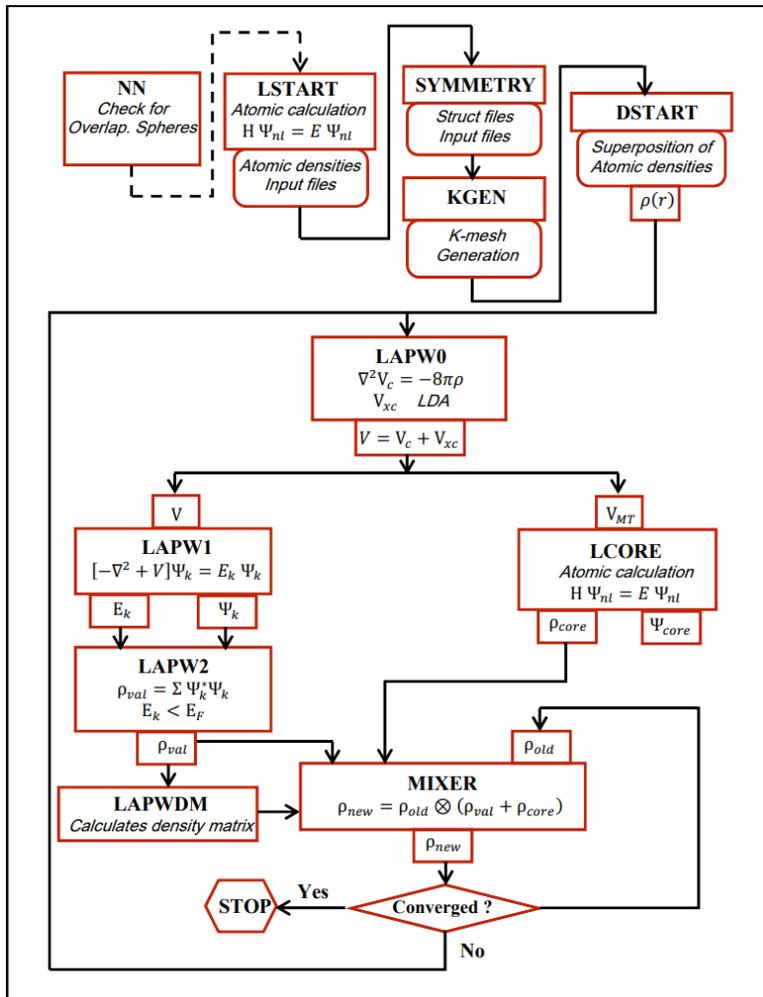


Figure 3.2: Work flow of the implementation of the SCF cycle in WIEN2k. [13]

The SCF cycle consists of a number of steps:

1. lapwo: calculates Columbic and exchange and correlational density
2. lapw1: calculates valence bands at all specified k-points
3. lapw2: valence electron densities calculated
4. lcore: core densities calculated
5. MIXER: combines core and valence densities

Additionally, there are some other key parameters that need to be considered before performing the convergence calculation: the convergence criteria. Here, we must consider the below.

*rk<sub>max</sub>*

The product of the smallest Muffin Tin Sphere (MTS) radius, and the largest  $K$  vector, yield the *rk<sub>max</sub>*. This quantity governs where electrons are treated as atomic-like functions (inside the spheres) or as plane-waves outside the sphere. In this thesis, the *rk<sub>max</sub>* value is set to 7 where otherwise noted.

### **K-point selection**

K-points are discrete points in the BZ and are used to sample the reciprocal space of the lattice. A commonly used K-point sampling scheme is the Monkhorst-Pack grid [15] and the Gamma-centered mesh. The Monkhorst-Pack grid is often used for materials with high symmetry, while the Gamma-centered mesh is preferred for systems with lower symmetry. For the work done in Wien2k in this thesis, I've used 1000 K-points as a compromise between accuracy and providing a convergence criteria that is reached within reasonable time.

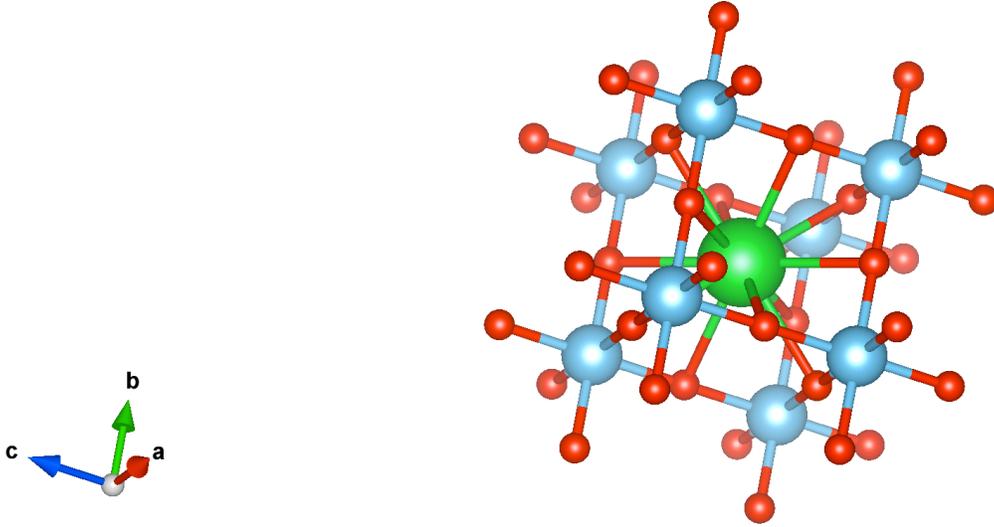


Figure 3.3: STO unit cell diagrammatic representation. Sr atom shown in green in the middle, surrounded by Ti atoms shown in blue. The lattice constant is known to be  $3.905\text{\AA}$  at room temperature,  $300\text{K}$ . Image produced in the VESTA software [16]

## 3.2 Strontium Titanate

Strontium Titanate,  $\text{SrTiO}_3$  or STO is a cubic phase perovskite at room temperature, belonging to the  $Pm\bar{3}m$  space group. The unit cell of STO is shown in Fig. 3.3. While very rare, STO occurs naturally in intrusive igneous rocks first discovered in Yakutia, Russia, and has since also been discovered in South America among other locations.

A well studied thermoelectric material, STO and its oxides are promising materials in the present day due to their thermoelectric and electronic properties. Oxides of perovskites have shown promising results as photovoltaic cells and come with the added advantages of lower costs and reduced dependence on rare earth metals that are difficult to mine and the processes are damaging to the environment.

The experimentally measured direct band gap in STO is  $3.75\text{eV}$  while the indirect band gap is known to be  $3.25\text{eV}$  [17]. Fig. 3.4 shows the com-

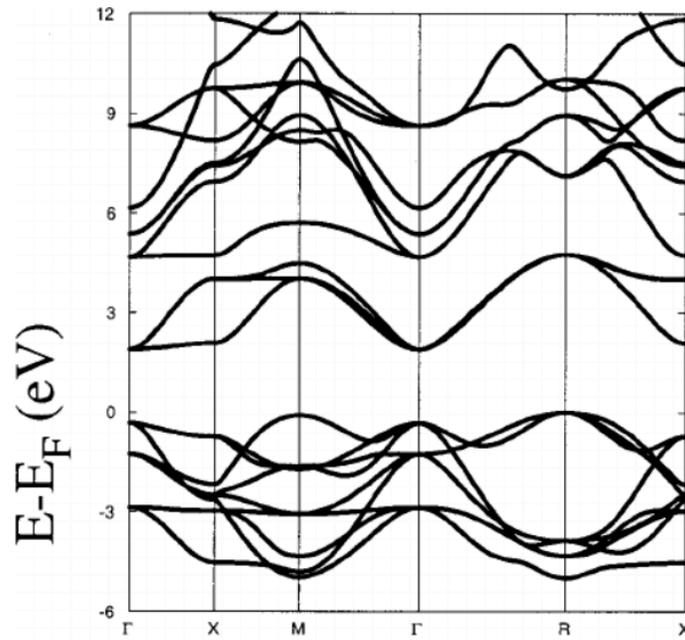


Figure 3.4: STO electronic band structure from literature using DFT with the Local Density Approximation [17]

putationally calculated band structure of STO using DFT.

With a split bonding character of both, covalent and ionic bonding, this gives rise to some interesting electronic properties. We can also see that there is a considerable energy gap between the conduction and valence bands.

## 3.3 Experimental Methods

### 3.3.1 Neutron Spectroscopy

Spectroscopy using neutrons is a well known and time-tested methodology. The principles that make it possible are derived from a number of disciplines in physics. Here, we will provide a short overview of inelastic neutron scattering (INS) and triple axis spectrometry.

### 3.3.2 The Scattering Cross Section

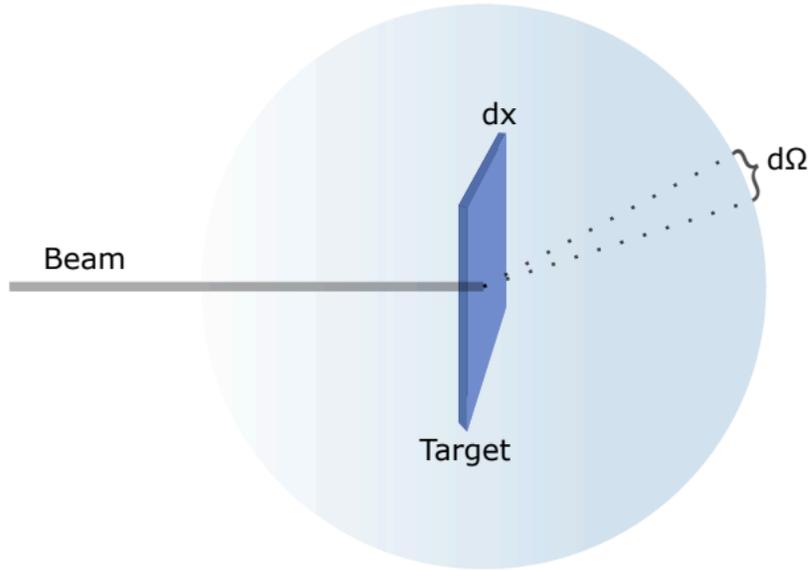


Figure 3.5: Scattering cross section

The flux  $\Psi$  of a beam of particles is given by the number of particles traversing a unit area per second. Beam particles encountering the target then scatter off in the three dimensional blue sphere as shown in Fig. 3.5.  $\sigma$  indicates the cross section, in units of Barn ( $1 \text{ Barn} = 10^{-28} \text{ m}^2$ ).

The double differential cross section  $d\sigma^2$  is obtained if we consider the number of particles scattered per unit time through a particular solid angle  $\Omega$  of a particular energy. We can find the differential cross section by integrating the  $d\sigma$  over all solid angles [18]. This yields the below double diffraction cross section expression at the heart of neutron scattering:

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} S(Q, E) \frac{\sigma}{4\pi} \quad (3.1)$$

With  $E_f$  is the scattered neutron energy, and  $S(Q, E)$  is the scattering function representing the physical quantity we are interested in.

### 3.3.3 Inelastic Neutron Scattering (INS)

During certain neutron scattering events, the neutrons either deposit energy into the target, or absorb energy from it. Therefore, in inelastic neutron scattering, we can write the energy transfer:

$$\bar{h}\omega = E_i - E_f = \frac{\bar{h}^2(k_i^2 - k_f^2)}{2m_n} \quad (3.2)$$

Then, in the quantum mechanical picture, we can describe the initial and final sample states as  $|\lambda_i\rangle$  and  $|\lambda_f\rangle$ . Now we write the double differential cross section:

$$\left. \frac{d^2\sigma}{d\Omega dE_f} \right|_{\lambda_i \rightarrow \lambda_f} = \frac{k_f}{k_i} \left( \frac{m_n}{2\pi\bar{h}^2} \right)^2 \left| \langle \lambda_i \psi_i | \hat{V} | \psi_f \lambda_f \rangle \right|^2 \delta(E_{\lambda_i} - E_{\lambda_f} + \bar{h}\omega) \quad (3.3)$$

$\hat{V}$  is the potential, and  $m_n$  the mass of the neutron. [18]

Here, we have some pre-factors, crossed with Fermi's Golden Rule (transition probability), crossed with an expression for energy conservation.

### Neutron Intensity, Scattering Length and Dynamic Structure Factor

Total neutron scattered intensity refers to the number of neutrons per unit area per unit time that are detected after a neutron scattering events. Neutron scattering as a probing technique, is limited by the intensity of the neutron beam encountering the sample, or incident flux.

Final measured intensity can be attenuated at a number of points in an instrument: source, moderator (brilliance), neutron guide, and even at the detector. The sample itself can also affect intensity since each material has a unique neutron scattering cross section. Plus, the thickness and material properties of the sample also impacts what fraction of incident neutrons are absorbed.

### 3.3.4 The Dynamic Structure Factor $S(Q, E)$

In neutron scattering experiments, the dynamic structure factor (DSF) is a key quantity that is a measure of scattering intensity as a function of both the momentum transfer  $Q$  and the energy  $E$ . This is a measurable quantity in INS experiments. The difference between the incident and scattered wavevectors gives the momentum transfer, and similarly the differences in incident and measured neutron energies can be calculated.

$S(Q, E)$  is a measure of the probability of discovering phonons at a specific momentum and energy transfer. The shape and form of the DSF can give information about lattice dynamics, structural and vibrational properties. The dynamic structure factor  $S(q, \omega)$  is a crucially important quantity that describes neutron scattering off a sample as a function of energy and momentum transfer. In inelastic neutron scattering experiments, the dynamic structure factor is measured by detecting the scattered neutrons and analyzing their energy and momentum transfers, and contains a wealth of information about interactions and correlations within a material.

$$S(\mathbf{Q}, \omega) = \frac{1}{2} \sum_{\nu} |F(\mathbf{Q}, \nu)|^2 \left( n_{\mathbf{q}\nu} + \frac{1}{2} \pm \frac{1}{2} \right) \delta(\omega \mp \omega_{\mathbf{q}\nu}) \quad (3.4)$$

The upper and lower signs refer to the creation and annihilation operators for an excitation such as a phonon, and the  $n_{\mathbf{q}\nu}$  is the Bose population function [19].

### 3.3.5 The phonon cross section

The inelastic scattering cross section for phonons is an important quantity that describes the probability of a phonon undergoing a change in energy or momentum in the scattering process.

Assuming a Bravais lattice, an expression for the phonon scattering

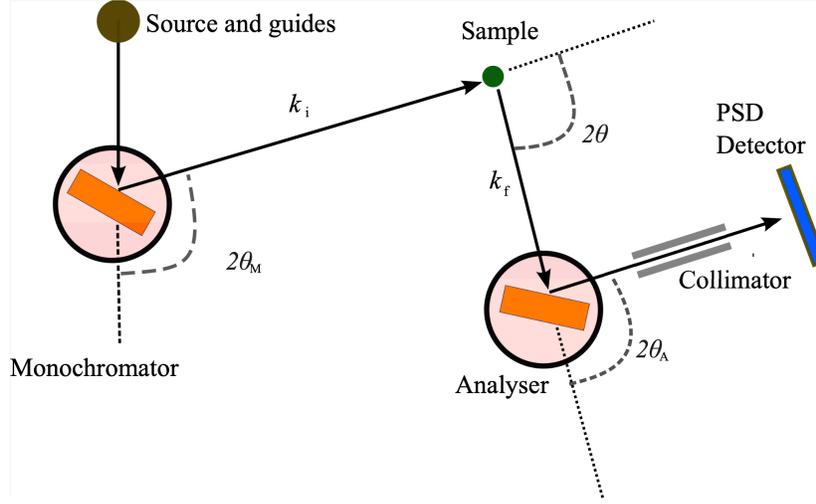


Figure 3.6: Schematic of the three axes of a TAS instrument [18]

cross section is given below [18]:

$$\left. \frac{d^2\sigma}{d\Omega dE_f} \right|_{\text{Bravais}} = \frac{k_f}{k_i} \frac{Nb^2}{2\pi\hbar} \exp(\langle U^2 \rangle) \times \sum_j \exp(i\mathbf{q} \cdot \mathbf{r}_j) \int_{-\infty}^{\infty} \exp(\langle UV \rangle) \exp(-i\omega t) dt. \quad (3.5)$$

$N$  is the number of independent oscillator modes, or phonons in this case.  $b$  is the neutron scattering length,  $U$  the harmonic oscillator operator,  $\exp(\langle UV \rangle)$  is an operator that creates and annihilates phonons.  $q$  is of course, the wave number, and  $r_j$  the deviation from equilibrium of the  $j$ -th atom.

### 3.3.6 The CAMEA Instrument

CAMEA is a multiplexing triple axis spectrometer (TAS) at the Paul Scherrer Institute in Switzerland [21]. TASs are particularly useful for our purposes as they are appropriate for measuring scattered neutron energy and momenta very precisely. Making use of Bragg's law:

$$n\lambda = 2d\sin(\theta) \quad (3.6)$$

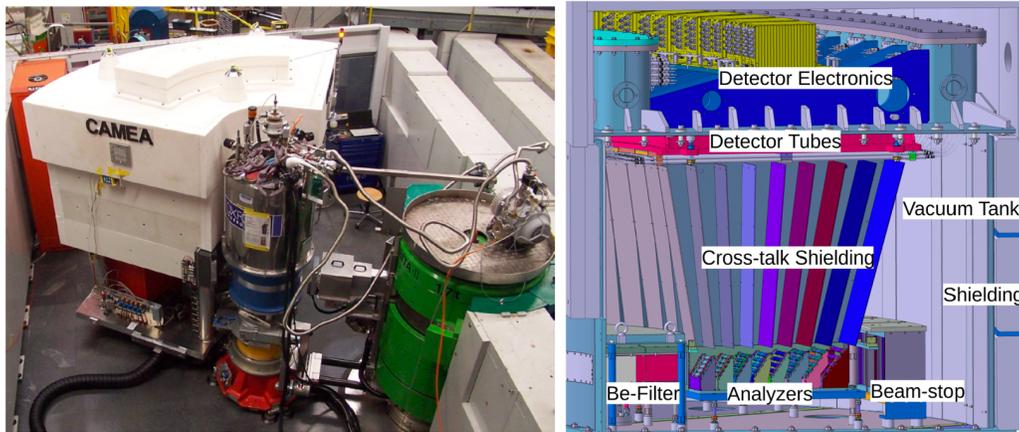


Figure 3.7: CAMEA Instrument and schematic [20]

incident neutron wavevectors are selected by Bragg reflections on a single crystal monochromator. The user can select from any wavevector fulfilling the Bragg condition by varying the scattering angle  $\theta$ .

### 3.3.7 Components of a Neutron Spectrometer

1. Source and guides: Typically a spallation or a reactor source. The PSI uses neutrons from a spallation source.
2. Monochromator: This is the energy resolution controller and is used to select neutrons of certain energies.
3. Sample: The sample to be analysed. Single crystal or a powder sample.
4. Analyser: Diffracts scattered neutrons of a specific energy, allowing only neutrons with the desired energy to reach the detector.
5. Collimator: Generally, defines the size and shape of the neutron beam—typically made of a hydrogenous neutron absorbing material to decrease background noise and to improve the signal-to-noise ratio.

6. Detector: The termination point of scattered neutrons where their dynamic properties and energy are measured. In CAMEA, there is a large detector bank made up of tubes filled with pressurised helium gas.

## 3.4 Theoretical underpinnings of the computational methods

### 3.4.1 The plane-wave method

Bloch's theorem states that electron wavefunctions in a periodic potential must be of the form:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r}) \quad (3.7)$$

The plane-wave method is primarily a basis set methodology where electronic wavefunctions are expanded in a set of plane waves [22]. Electron wavefunctions are expanded in a Fourier series of plane waves, which are periodic functions with a fixed wavelength and wavevector. This expansion also satisfies the periodic boundary conditions and is therefore an efficient method for calculating properties of interest. In a system where electrons obey Bloch's Theorem, we can expand the electronic wavefunction as

$$\Psi(\mathbf{r}) = \sum_G C_G e^{i\mathbf{G}\cdot\mathbf{r}} \quad (3.8)$$

Here  $\Psi(r)$  is the wave function at position  $r$ ,  $G$  is a vector in reciprocal space,  $C_G$  is the coefficient of the plane wave with wavevector  $G$ . The coefficients are obtained from solving the Kohn-Sham equations that we encountered earlier.

However, in practice, we cannot work with an infinite basis set and so we need a limitation. For plane waves, this is an easy task as we can limit the set to all  $G$  where  $G < G_{max}$  - a sphere of radius  $G_{max}$  and all reciprocal lattice vectors are in the basis set. Now I term the corresponding energy

the cutoff energy:

$$E_{cut} = \frac{\hbar^2}{2m} G_{max} \quad (3.9)$$

Usually cutoff energies are in the range of  $20 - 200 Ry$  depending on the system and convergence criteria.

For the purposes of testing and benchmarking, Titanium Carbide (TiC) was used. The structure Crystallographic Information File (CIF) for TiC was downloaded from MaterialsProject [23]. Upon following the aforementioned self consistency scheme, the densities of states plots and phonon dispersion figures were generated and plotted in Wien2k. Comparing with known DOS and phonon dispersion plots for TiC, it was determined that all systems in Wien2k were running nominally.

## 3.5 Computational Calculation Software

### 3.5.1 Quantum Espresso

Espresso is an acronym that stands for OPEN Source Package for Research in Electronic Structure. Quantum Espresso is an integrated suite of computational simulation software that is capable of calculating electronic structure, and modeling of materials. It is based on the plane-wave basis set pseudopotential method and is suitable for performing ground-state calculations, optimising structures, and other inquiries into the nature of materials [22].

Pseudopotentials are a powerful DFT calculational tool that allow one to replace the electron-ion interaction potential with a simpler, effective potential that approximates the true potential but requires fewer electronic states to be included in the calculations. For the sake of optimising computational complexity, in describing structural dynamics, core electrons are not active participants in the description of electronic properties, and therefore we are nudged towards trying to approximate the wavefunctions near the nuclei. Plane wave pseudopotentials are often combined with the frozen core approximation which are employed to ensure consistency in

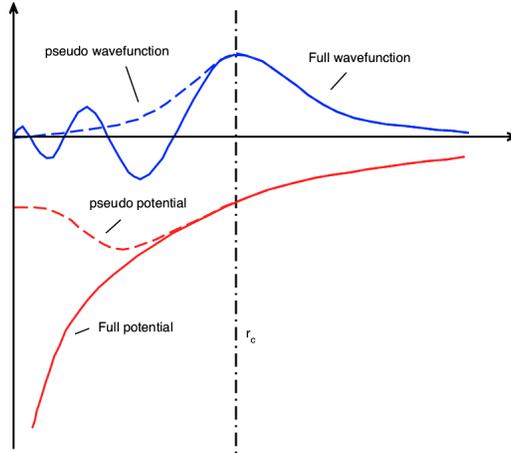


Figure 3.8: Graphical illustration of the pseudopotential concept [24]

the dynamics of the core electrons.

For my investigations of STO, I used projector augmented wave (PAW) pseudopotentials as they are suitable for my perovskite material. Ultra-soft pseudopotentials (USPPs) are also available and supported by QE, however in this thesis, I use solely PAW pseudopotentials.

The primary QE framework I'm executing in this thesis is the *pw.x* script that executes a planewave self-consistent calculation.

### The Pseudopotential Method

QE requires pseudopotentials to be delivered in the Unified Pseudopotential Format (UPF). For my investigation of STO, I obtained PAW pseudopotential files for strontium, titanium and oxygen from the Standard solid-state Pseudopotentials (SSSP) library on Materials Cloud - which is a publicly available resource. [25]

#### 3.5.2 QE Input file

Running the *pw.x* program on Quantum Espresso suite requires the user to first prepare an input file, also known as a control file. Here, we specify basic structural information about the material being studied. This com-

mand then performs a self-consistency DFT calculation and outputs a file which describes a wavefunction of the system that we inputted.

The QE input file is a plaintext file consisting of a number of name-cards beginning with the ampersand symbol and separated by a forward slash.

```
&CONTROL
calculation = 'scf'
Prefix = 'paw'
pseudo_dir = '.'

/
&SYSTEM
ibrav = 1
A=3.91
nat=5
ntyp=3
ecutwfc=30
/
&ELECTRONS
/

ATOMIC_SPECIES
Sr 87.620 Sr_pbe_v1.uspp.F.UPF
Ti 47.867ti_pbe_v1.4.uspp.F.UPF
O 15.999 O.pbe-n-kjpaw_psl.0.1.UPF

ATOMIC_POSITIONS {crystal}
Sr      0.0000000000    0.0000000000    0.0000000000
Ti      0.5000000000    0.5000000000    0.5000000000
O       0.5000000000    0.0000000000    0.5000000000
O       0.5000000000    0.5000000000    0.0000000000
O       0.0000000000    0.5000000000    0.5000000000
```

```
K_POINTS {automatic}
16      16      16
```

The *control* card defines the type of calculation, where the output files will be returned, and the pseudopotential file path.

In *system* we input the symmetries of the lattice, the lattice constant, the number of atoms and the number of atomic species. We also specify *ecutfcw* which is the kinetic energy cutoff of the wavefunction in units of Ry.

*ATOMIC SPECIES* defines the elements present, and the names of their respective pseudopotential files. Similarly, *ATOMIC POSITIONS* describes the fractional coordinates of atoms in our unit cell.

The first calculation I carried out was the SCF calculation for STO using the above input file. The calculation was carried out on the UiS remote server where parallel computing was possible, and up to 24 cores are available.

## 3.6 Phonopy

In order to implement the finite displacement method in our material, we invoke another well known software package, Phonopy [26]. The finite displacement method is a widely used first-principles method for calculating the phonon frequencies and eigenvectors of a crystal. The method is based on calculating the small energy differences that occur due to small displacements of atoms from their equilibrium positions. To achieve this, atoms in the supercell are displaced in each of the Cartesian directions by a fraction of an angstrom, while other atoms are fixed. We then calculated the energy of the supercell for each displacement using Quantum Espresso, and used finite difference techniques to calculate the second derivative of the energy with respect to the displacement. The second derivative is related to the force constant matrix of the material, and de-

scribes atomic coupling, and therefore phonon frequencies and eigenvectors.

Then the force constant matrix is fed into Phonopy where it computes phonon frequencies and eigenvectors in the Brillouin zone. We can then recover the phonon dispersion relation and density of state plots.

To begin with this method, we first generate a number of  $3 \times 3 \times 3$  supercells of STO with appropriate dimensionality and symmetry using Quantum Espresso.

# Chapter 4

## Results

The results we obtained are in equal parts intriguing and illustrative of the reasonable precision and utility of Density Functional Theory as a computational modelling tool. In this section we present and analyse results of computational and experimental work carried out throughout this thesis, and compare our results to published work. We shall be looking at computational calculations first, then later, we consider results from an inelastic neutron scattering experiment (INS), and compare the two.

We will begin by looking at the capabilities of WIEN2k in calculating electronic properties in a test material (titanium carbide) and then STO. Later, we turn to Quantum Espresso for the phonon character in STO using DFPT and the finite displacement (supercell method). Phonopy was then used for post-processing and preparing files for our final computational calculations package, Euphonic, where we produced the dynamic structure factor plot. Later, we present results from the INS experiment using CAMEA, and compare the two methodologies by analysing the results.

### 4.1 WIEN2k

TiC is a well studied cubic material with known electronic and thermal properties. Therefore it can act as an ideal benchmarking material to ensure that my WIEN2k code compiled correctly and that all required func-

tionality was working nominally.

The main electronic band structure of Titanium Carbide, TiC, was calculated using WIEN2k up to  $E = 8eV$ . This gives us the dispersion relation in TiC which is the relationship between the energy and wave vectors of the electrons. For this calculation, I used the standard Graduated Gradient Approximation XC functional. The calculation was spin-unpolarised, and as expected, there is no band gap in this material. The  $1s, 2s, 2p$  orbitals inhabit the spin core states and  $3d, 4s, 4p$  the valence states. Results from this calculation are shown in Fig. 4.1. We can see that the electronic bands cross the Fermi Energy level in TiC (no band-gap), and that's what we expect from a metallic material. In general we see that flatter bands in the electronic dispersion relation correspond to weaker orbital interaction energies, while more disperse bands denote stronger orbital interactions. We can compare these results to published band structure for TiC using PBE-GGA, under the plane wave method shown in Fig. 4.2 [27]. Accounting for the different paths through the Brillouin zone in the calculated and known electronic dispersion relation, we have broad agreement between two.

Additionally, Densities of state (DOS) is a measurement of the allowed energy states per unit volume and per unit energy in a material. Whereas, the projected/partial density of state plot describes the DOS of a specific subset of atoms or orbitals in the material. The Partial/Projected Densities of State (PDOS) plot for TiC obtained from WIEN2k is given in Fig. 4.3. Here we can see which atomic species are making relevant contributions at particular energy levels.

WIEN2k DOS and PDOS calculations were carried out for our materials between  $-5eV$  and  $8eV$ . The dotted line indicated the Fermi energy  $E_f$ , which has been set to zero.

### 4.1.1 Electronic Properties of STO using WIEN2k

Having validated the implementation of electron dispersion calculations in WIEN2K, we now turn our attention to the material we are interested in, SrTiO<sub>3</sub> and begin by looking at the Density of State (DOS) plot given in Fig. 4.4. The PDOS was also calculated using both, the PBE-GGA (Fig. 4.5) and the mBJ (Fig. 4.6) functionals as described in chapter 2.

We can see that in the valence band, oxygen has the highest contribution to the electronic properties, and Titanium has the highest contribution in the conduction band of STO. This is due to the fact that oxygen is more electronegative than strontium or titanium, and as such, oxygen tends to have a partial negative charge, and conversely Sr and Ti a partial positive charge, forming strong covalent bonds.

In the conduction band containing the lowest electronic energy states, Ti has a higher contribution due to weaker binding with its electrons - electropositivity. The factors at play are the extent of electronegativity, crystal structure in the cubic phase, and the kinds of interatomic bonding at play.

It is also apparent that, overall, the PBE-GGA functional DOS calculations underestimate the Strontium contributions in the both regions compared to the mBJ functional (Fig. 4.7). This can be attributed to the incorporation of electron-electron effects in the mBJ functional, and the inability of the PBE-GGA to capture the strong inter-electron correlations [28].

The electronic band structure for STO is given in Fig. 4.8 and Fig. 4.9 using both the PBE-GGA and the mBJ functions respectively. Here we can see that the mBJ functional yields a better approximation of the band gap in STO, which has been experimentally measured to be  $3.25\text{eV}$  using vacuum ultraviolet spectroscopy [29]. PBE-GGA suggests a band gap of  $2\text{eV}$ , while mBJ suggests  $3.8\text{eV}$ .

It is well known that the GGA functional underestimates band gaps, while the mBJ functional was conceived to contravene this very problem by incorporating corrections for self-interaction errors [30].

## 4.2 Quantum Espresso

Using plane wave basis sets, Quantum Espresso (QE) allows for quicker and more efficient DFT calculations for larger systems compared to WIEN2k. Since we are interested in both the electronic properties and the harmonic phonon approximation in STO, I continued my investigation by compiling and initialising Quantum Espresso on UiS's server cluster. The first step in our Quantum Espresso journey is to perform the *pw.x* self consistency calculation, once converged at the threshold specified by the user, yields a number of crucial parameters of interest. These include the total energy, the electronic density, the charge density and information about convergence: how many iterations were performed. In the end, we have our working wavefunction for the system.

### 4.2.1 Generating the ground-state wavefunction of STO

The SCF cycle as described earlier in the self consistency scheme solves the KS equations and returns a file that describes the ground state energy of the system. QE performed 19 iterations and lists the below energy information about our STO unit cell:

```
highest occupied level (ev):      9.8260

total energy                      =   -562.35624228 Ry
total all-electron energy         =   -8511.816462 Ry
estimated scf accuracy           <    0.00000018 Ry
```

The total energy is the sum of the following terms:

```
one-electron contribution         =   -72.82365932 Ry
hartree contribution              =    60.59665902 Ry
xc contribution                    =   -58.88529594 Ry
ewald contribution                 =  -212.23504729 Ry
```

```
one-center paw contrib. = -279.00889876 Ry
```

Now that we have performed the *pw.x* calculation, we are ready to continue on to optimising the structure, and to describe phonon properties in STO.

### 4.2.2 Optimising the structure of STO

When optimising the structure of a material in Quantum Espresso, we are basically searching for the arrangement of atoms in such a way that it minimises the total energy of the system: a system at zero pressure and temperature. It is a necessary step before we begin working out electronic properties and lattice dynamics. QE performs a series of iterative calculations to determine the most stable configurations of atoms in the unit cell. The process starts with an ansatz wavefunction of the system that is continuously refined until the total energy reaches a minimum.

To begin optimisation in QE, we create an optimisation control file which is similar to the structure control file described in the Methods section, but rather than an SCF calculation, we choose the *vc-relax* option which allows both the atomic positions and the lattice constant to vary. *vc-relax* also allows for the stress tensor to be calculated and this is an important component in the upcoming phonon calculations.

Then we perform the *pw.x* plane wave calculation and upon convergence, we obtain a new optimised structure output file. The input file is given below:

```
&CONTROL
calculation = 'vc-relax'
restart_mode = 'restart'
prefix = 'shiblrelax'
pseudo_dir = '.'
forc_conv_thr=1d-5
nstep=1000
```

```

/
&SYSTEM
ibrav = 1
nat=5
ntyp=3
ecutrho = 300
ecutwfc=39
cellldm(1) = 7.38
/
&ELECTRONS
/
&IONS
ion_dynamics = 'bfgs'
/
&CELL
cell_dynamics = 'bfgs'
/
ATOMIC_SPECIES
Sr 87.620 Sr.pbesol-spn-kjpaw_psl.1.1.0.0.UPF
Ti 47.867 Ti.pbesol-spn-kjpaw_psl.1.1.0.0.UPF
O 15.999 O.pbesol-n-kjpaw_psl.1.1.0.0.UPF

ATOMIC_POSITIONS {alat}
Sr      0.0000000000    0.0000000000    0.0000000000
Ti      0.5000000000    0.5000000000    0.5000000000
O       0.5000000000    0.0000000000    0.5000000000
O       0.5000000000    0.5000000000    0.0000000000
O       0.0000000000    0.5000000000    0.5000000000

K_POINTS {automatic}
9 9 9 0 0 0

```

After a period of time, QE returned the optimised structure output file,  
with results of interest shown below:

Final enthalpy = -562.3602618000 Ry

Begin final coordinates

new unit-cell volume = 388.61505 a.u.<sup>3</sup> ( 57.58681 Ang<sup>3</sup> )  
density = 5.29084 g/cm<sup>3</sup>

CELL\_PARAMETERS (alat= 7.38000000)

0.988819095	0.000000000	0.000000000
0.000000000	0.988819095	0.000000000
0.000000000	0.000000000	0.988819095

ATOMIC\_POSITIONS (alat)

Sr	0.000000000	0.000000000	0.000000000
Ti	0.4944095476	0.4944095476	0.4944095476
O	0.4944095476	0.000000000	0.4944095476
O	0.4944095476	0.4944095476	0.000000000
O	0.000000000	0.4944095476	0.4944095476

Note that 1 Å= 1.89A.U If we compare these results to our unrelaxed structure:

bravais-lattice index = 1  
lattice parameter (alat) = 7.3888 a.u.  
unit-cell volume = 403.3916 (a.u.)<sup>3</sup>

ATOMIC\_POSITIONS {alat}

Sr	0.000000000	0.000000000	0.000000000
Ti	0.500000000	0.500000000	0.500000000
O	0.500000000	0.000000000	0.500000000
O	0.500000000	0.500000000	0.000000000
O	0.000000000	0.500000000	0.500000000

We can see above and in Fig. 4.10 that the unit-cell volume has dropped from  $403.392a.u^3$  to  $388.62a.u^3$ , and the atomic positions have been changed, as expected. These atomic coordinates now represent the relaxed configuration of STO. The experimentally measured volume of STO has been determined to be  $59.5 \text{ \AA}^3 = 399.4a.u^3$ . This measurement was done by Muhammad et al using powder X-ray diffraction [31].

### 4.2.3 Phonon modes at the gamma point

The Gamma point ( $\Gamma$ ) is the point in the middle of the Brillouin zone and that is where the momentum transfer,  $Q$  is zero. Since we have five atoms in the basic unit cell of STO, we expect there to be  $3 * 5 = 15$  phonon eigenmodes, although some of them are degenerate (overlapping) modes. We can see below in the QE output, there are some modes with negative frequencies that are unphysical. We can postulate that these modes are the result of numerical inaccuracies arising from the underlying XC functional, and can be corrected by considering anharmonic phonon terms.

```
*****
freq ( 1) =      -3.677177 [THz] =      -122.657424 [cm-1]
freq ( 2) =      -3.677177 [THz] =      -122.657424 [cm-1]
freq ( 3) =      -3.677177 [THz] =      -122.657424 [cm-1]
freq ( 4) =       3.715090 [THz] =       123.922048 [cm-1]
freq ( 5) =       3.715090 [THz] =       123.922048 [cm-1]
freq ( 6) =       3.715090 [THz] =       123.922048 [cm-1]
freq ( 7) =      12.357525 [THz] =      412.202660 [cm-1]
freq ( 8) =      12.357525 [THz] =      412.202660 [cm-1]
freq ( 9) =      12.357525 [THz] =      412.202660 [cm-1]
freq (10) =      12.760598 [THz] =      425.647723 [cm-1]
freq (11) =      12.760598 [THz] =      425.647723 [cm-1]
freq (12) =      12.760598 [THz] =      425.647723 [cm-1]
freq (13) =      13.281363 [THz] =      443.018568 [cm-1]
freq (14) =      13.281363 [THz] =      443.018568 [cm-1]
```

$$\text{freq} ( 15) = 24.304812 \text{ [THz]} = 810.721272 \text{ [cm-1]}$$

\*\*\*\*\*

The higher frequency modes are optical modes, whereas at the gamma point, we expect the acoustic modes to be at lower frequencies - nearly zero. We see reasonable agreement when comparing these results to the Phonon Database phonon dispersion relation shown below in Fig. 4.11 [32].

Then using Density Functional Perturbation Theory (DFPT), mentioned in the Background section, we work towards producing the DOS and phonon dispersion plots using Quantum Espresso and Phonopy.

### 4.3 Experimental Results

My thesis advisor Dr. Diana Lucia Quintero and her team from the aforementioned PHUN project (Roshaninejad, Kadamane, Kojda and Habicht) along with instrumentalist J. Lass, performed an inelastic neutron scattering experiment using the Continuous Angle Multiple Energy Analysis (CAMEA) instrument at the Paul Scherrer Institute (PSI), observing phonon modes in STO at 115K and 300K within the [H,H,L] plane, and obtained phonon dispersion diagrams. As previously states, in this thesis, we are concerning ourselves with a purely harmonic phononic approximation, whereas a Triple Axis Spectrometer such as CAMEA, of course, provides a full spectrum of phonon effects up to  $8meV$ . We will compare our *ab initio* DFT calculations with neutron scattering results and discuss where and how the harmonic *ab initio* approximation is a valid proxy for experiment, and conversely, where it fails to reproduce experimental results in their totality.

The experiment used inelastic neutron scattering and the sample size was  $20mm * 10mm * 10mm$ . Their results are given in Fig. 4.13 and Fig. 4.14. This is a lateral constant energy 2D cut of the 3D neutron scattering data ( $[H, H, L], \nabla E$ ), a constant  $q$ -direction versus energy transfer. Fig.

4.13 shows phonon dispersion around the centre of the Brillouin zone (the  $\Gamma$  point) and other high symmetry points in the BZ. Fig. 4.14 is a slice through one of these special k-paths in lighter colours, and weaker intensity at the  $R$  point. The colour of the curve corresponds to neutron intensity.

## 4.4 DFPT and Phonopy

Using the DFPT method, it is possible to obtain phonon dispersion diagrams for STO. Fig. 4.15 shows the phonon dispersion calculated using the DFPT method in Quantum Espresso, and then post processed using Phonopy, and plotted using Python. Fig. 4.12 shows the BZ of STO in XCrystDen and are able to identify the fractional coordinates of the  $\Gamma$  and  $M$  points. These were then used in Euphonic to plot the phonon dispersion along a specified direction. Euphonic is an inelastic neutron scattering simulation tool that is able to work with force constant matrix datasets from Phonopy or Quantum Espresso to produce results comparable to INS experiments [19].

The Q-path was chosen as  $\Gamma \rightarrow M \rightarrow \Gamma$

In Fig. 4.15, we can see that we primarily have transverse optical modes in the higher energy range, and both, transverse acoustic and longitudinal acoustic modes in the lower energy range.

### 4.4.1 The Supercell method to determine additional properties

In order to determine the Dynamic Structure Factor using the Euphonic software package, we are currently limited to using the finite displacement method to create supercells of our material. Using Quantum Espresso to create a set of 8 distinct  $3 \times 3 \times 3$  supercells of STO (135 atoms each), along with the corresponding force sets file, this information is then passed on to Euphonic for neutron scattering intensities and structure factor calcu-

lation.

Euphonic is a Python based tool that works with output files from Phonopy or CASTEP. Using the finite displacement method, it is possible to produce dynamic structure factor  $S(Q, \omega)$  plots in Euphonic along K-paths in the Brillouin zone. It allows us to simulate an inelastic neutron scattering experiment given a certain material.

The neutron scattering cross section, as we have seen it earlier, given in terms of the  $S(Q, \omega)$ :

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} S(\mathbf{Q}, \omega) \quad (4.1)$$

Within the energy range the experiment was carried out in, we have agreement between INS results and calculational results.

#### **4.4.2 Comparing DFT calculations with experimental results**

In this thesis we are concerned with comparing the efficacy of DFT (and its derivative computational modelling methods) with experimental INS in the study of the harmonic phonon approximation. This should give us further information about the accuracy of the computational methods, their shortcomings, and also allow us to learn more about phonon transport in STO.

Looking at Fig. 4.15, it is possible to again ascertain that the higher energy modes are optical phonons whereas acoustic modes occupy lower energy levels.

If we overlay our figures, we can see that there is agreement between DFT calculation and neutron scattering data. This comparison is given in Fig. 4.18.

And so in Fig. 4.18, we can see the DFPT calculated phonon dispersion overlaid on top of CAMEA data (Fig. 4.13). This figure illustrates the

culmination of the essence of our investigation in our thesis: how well our computational model of the transport properties in STO corresponds with experimentally determined properties.

To make a fair comparison, the computed phonon dispersion curve had to be mirrored vertically so that it describes the  $\rightarrow M \rightarrow \Gamma$  path we have data for from CAMEA. Then, after some scaling of axes and figure alignment, we can see that there is agreement between computation and experiment in regards to one particular phonon mode. The computational data fits the experimentally produced curve quite well. The gradients match each other well and since this is one of the acoustic modes, the first derivative of this curve would yield the velocity of sound in the material.

The main handicap we encounter in the comparison is the maximum energy range (10 meV) achieved in the CAMEA experiment, whereas computational calculations allow us to reach arbitrarily high energies.

Since this particular phonon mode is comparatively lower in energy and exhibits negative curvature with lower dispersion, one can deduce that this is a transverse acoustic mode.

In the dynamic structure factor plots given in Fig. 4.16 and Fig. 4.17, the intensity is an indicator of the probability of exciting a phonon at a given momentum or energy. Intense and sharp peaks represent phonon modes with longer lifetimes - time taken to decay.

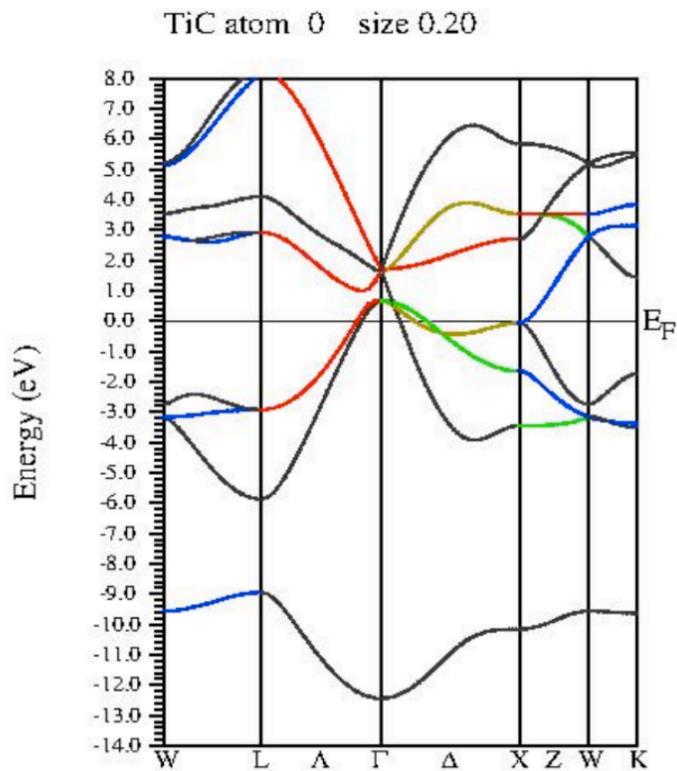


Figure 4.1: TiC electronic band structure drawn in the Linux based Xmgrace software suite. Plotted between  $-14eV$  and  $8eV$ . Fermi level shown as  $E_F$ . The line colours in the calculated plot do not have a physical meaning and are merely visual aids.

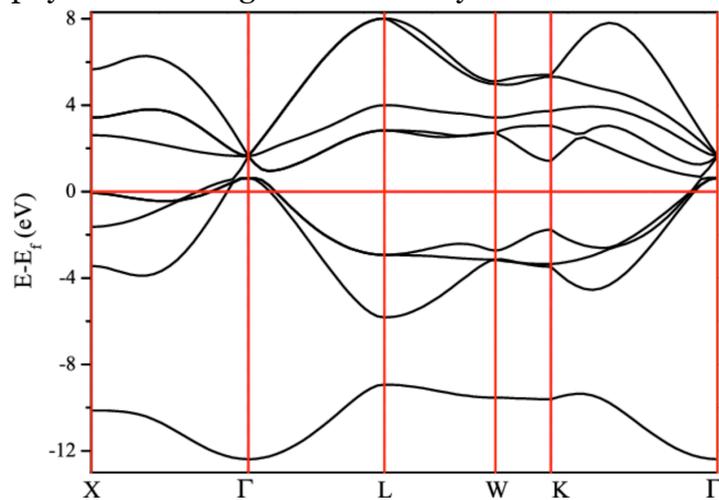


Figure 4.2: TiC Band Structure from literature, computationally calculated using the PBE-GGA functional [27]. We see good agreement with 4.1

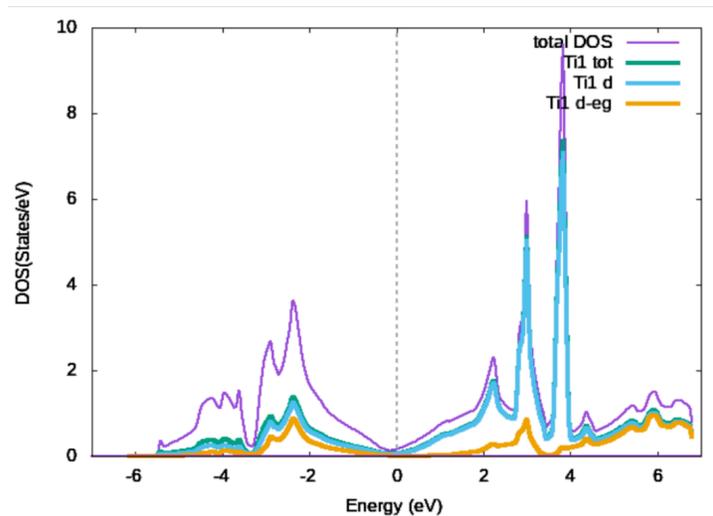


Figure 4.3: TiC DOS using the PBE-GGA functional: we can see that the  $d$  orbitals have the highest contribution in the valence band

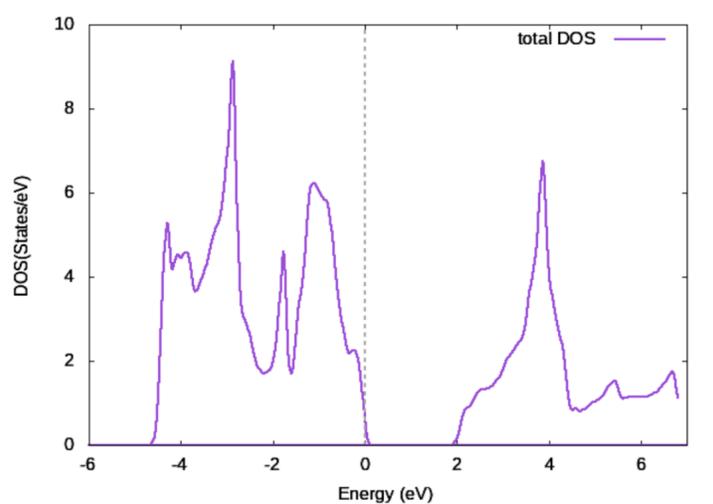


Figure 4.4: STO DOS using the PBE-GGA functional, energy given in  $eV$  on the x-axis, and number of states per  $eV$  on the y-axis

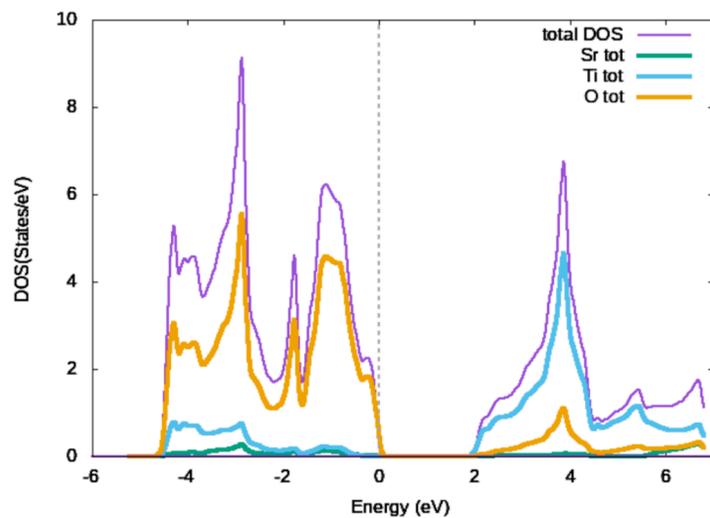


Figure 4.5: STO PDOS using the PBE-GGA functional, calculated in WIEN2k and plotted on Xm-Grace

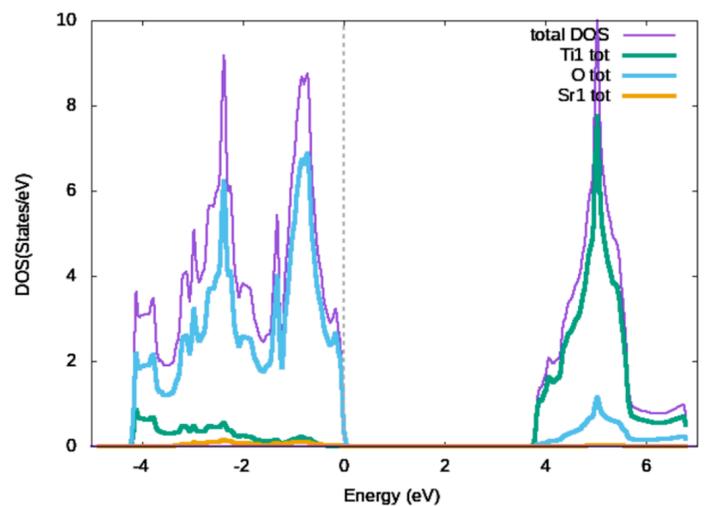


Figure 4.6: STO DOS with the mBJ functional

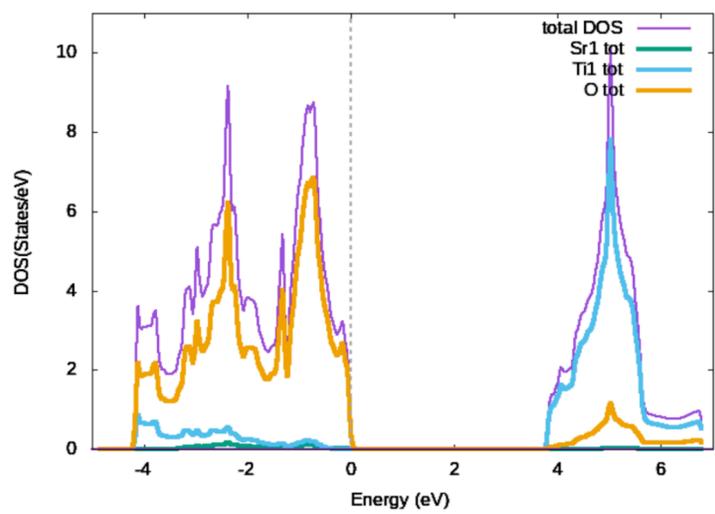


Figure 4.7: STO PDOS using the mBJ functional

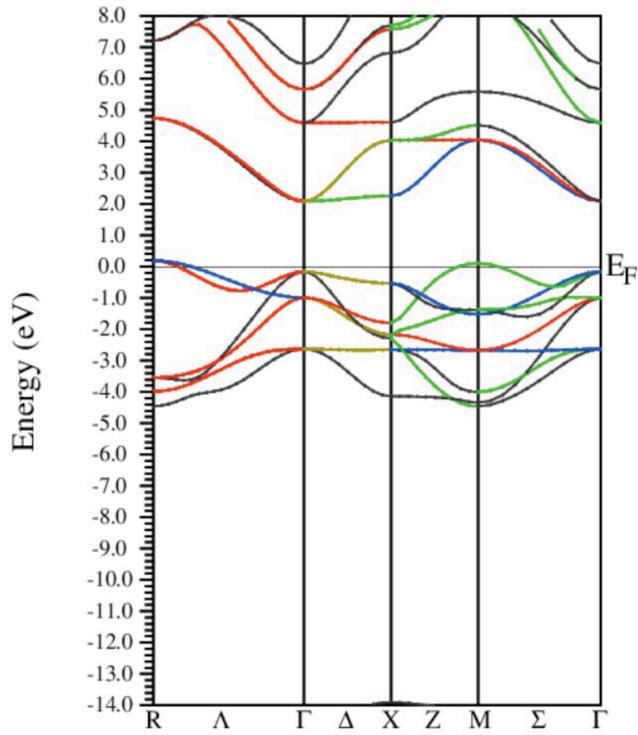


Figure 4.8: STO PBE-GGA band structure  
 titanmbj atom 0 size 0.20

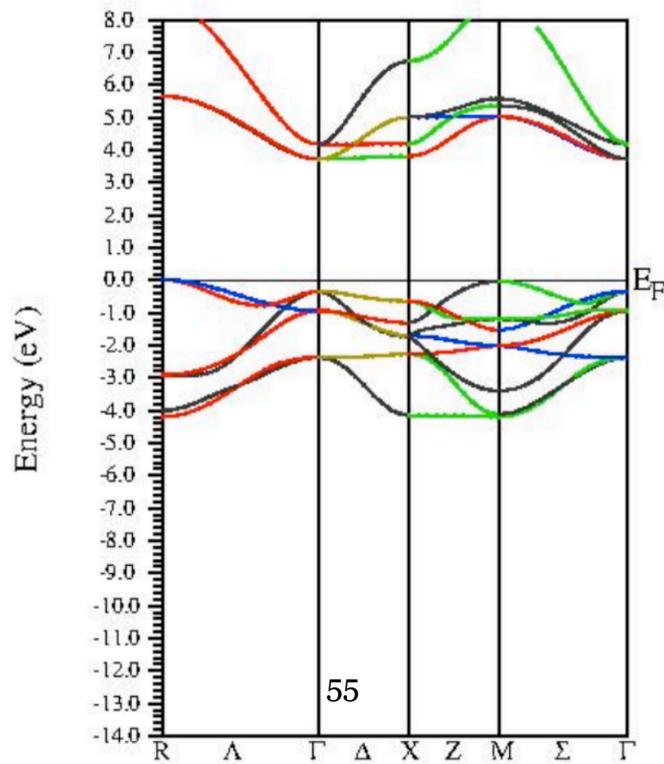


Figure 4.9: STO mBJ band structure

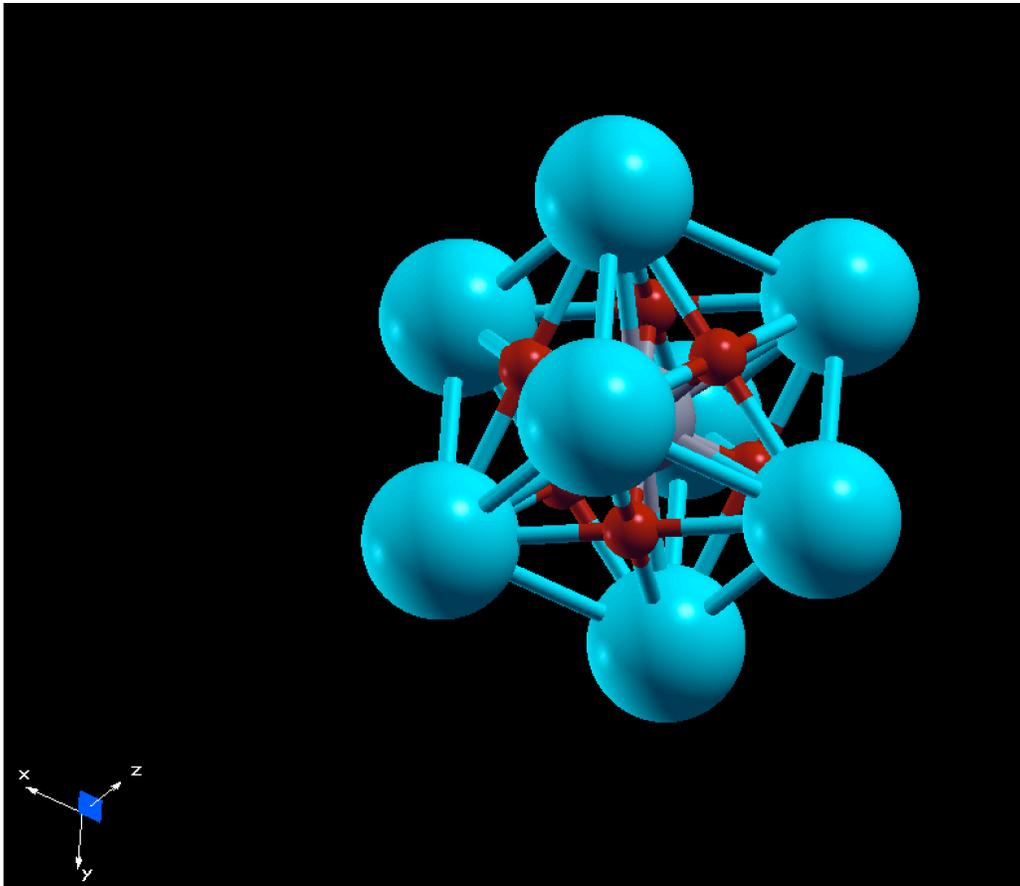


Figure 4.10: The relaxed structure of STO plotted on Xcrysden. We see Strontium Atoms on the corners of the unit cell with titanium in the middle.

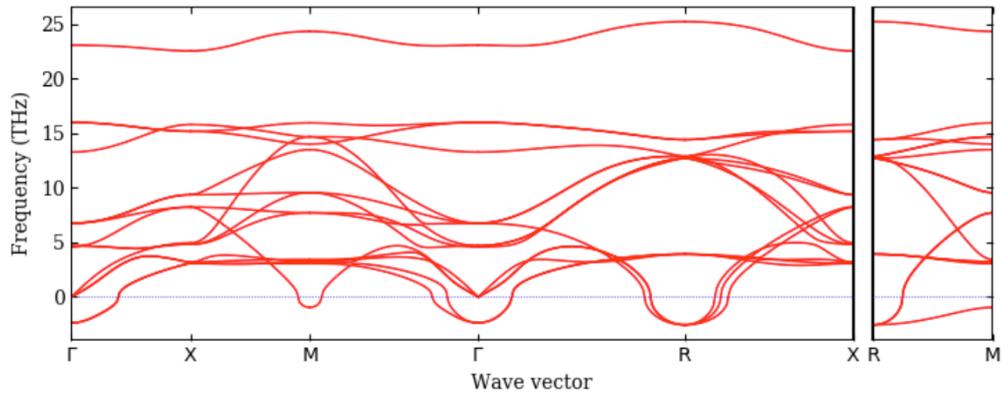


Figure 4.11: Known phonon dispersion in STO from literature. Note that here we are simply comparing the number of phonon modes. [32]

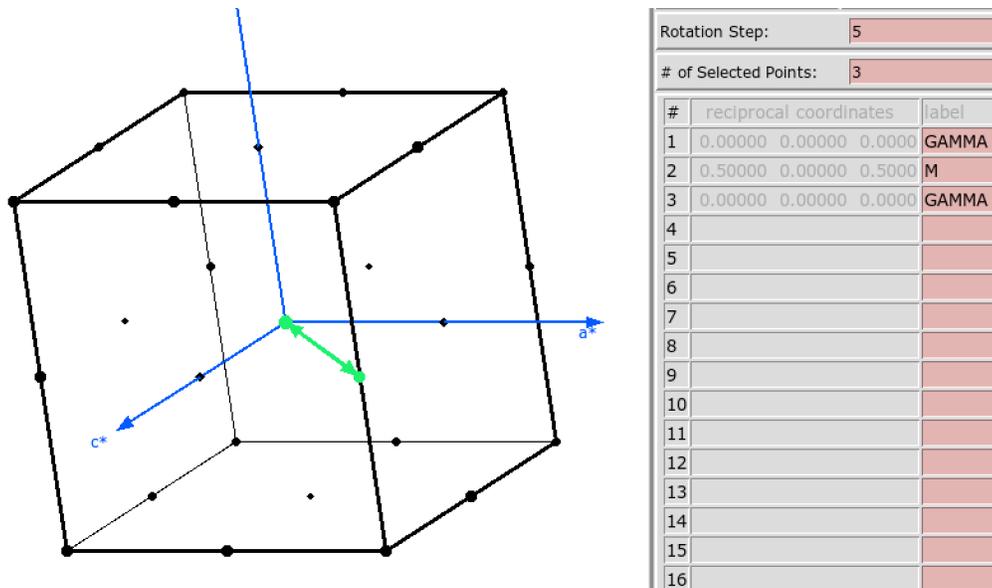


Figure 4.12: High symmetry points of interest in the STO Brillouin Zone - from Xcrysden

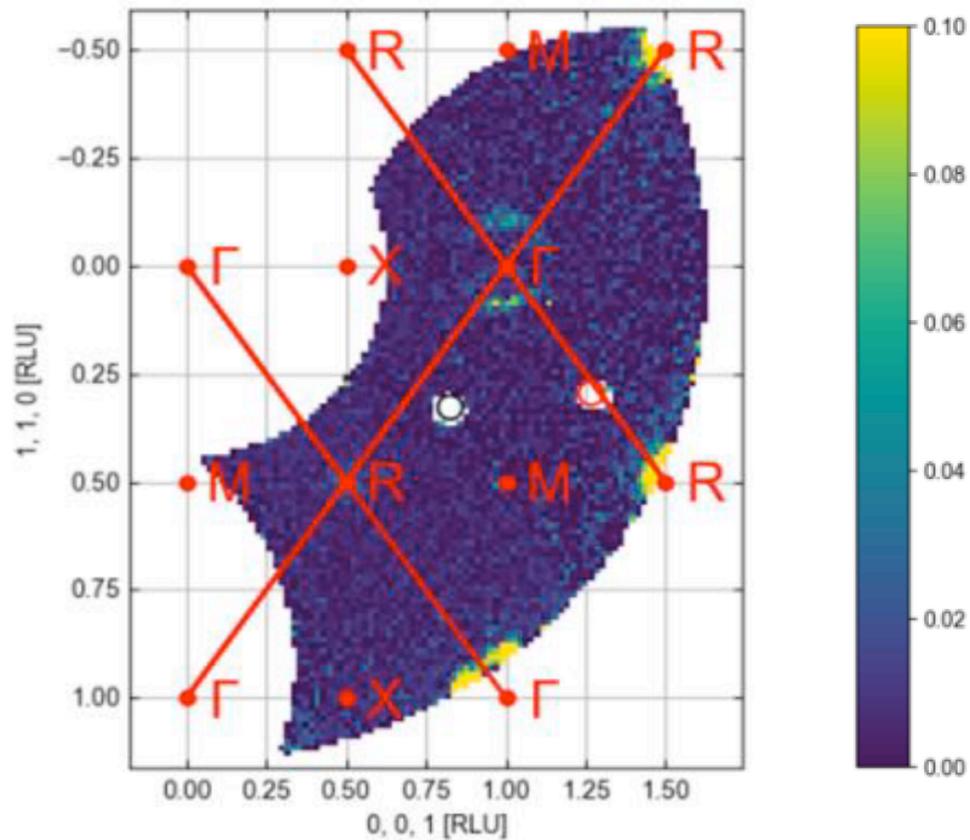


Figure 4.13: Q-E map of scattering intensities at a constant energy at  $6.1\text{meV}$ , with high symmetry directions overlaid - data from CAMEA. In the colour scale using arbitrary units, the more yellow regions denote higher neutron counts, and the darkest blue, zero neutron counts. Figure plotted on the Mjolnir Software package.

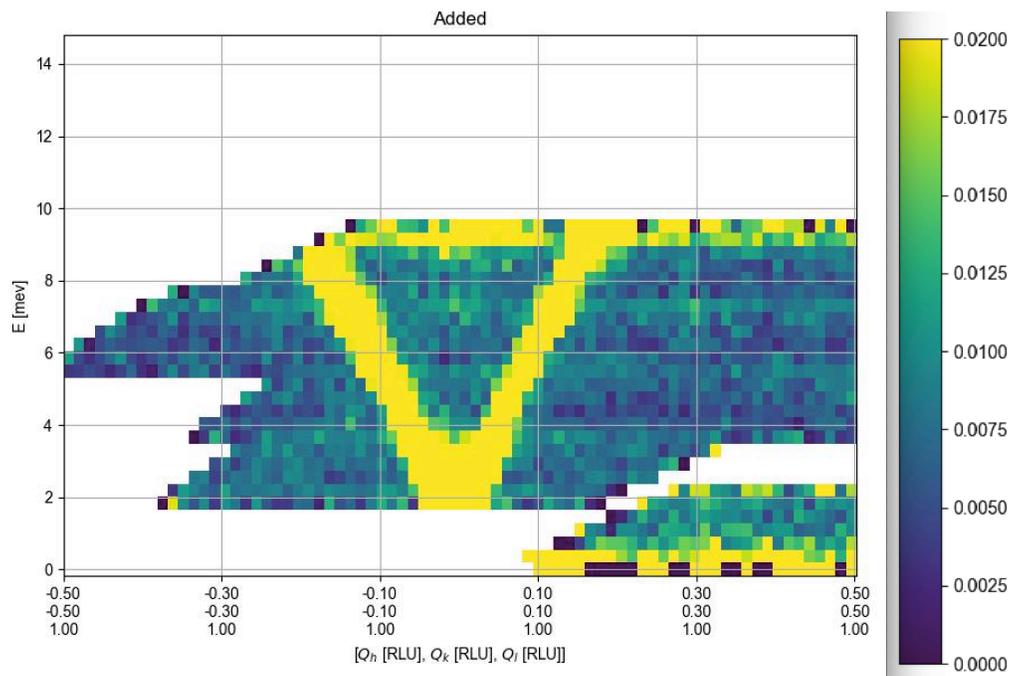


Figure 4.14: 2D cut of phonon dispersion along  $M \rightarrow \Gamma \rightarrow M$  in the (H,H,L) plane – data from CAMEA. The colour legend shows neutron counts in arbitrary units. Figure plotted on the Mjolnir Software package.

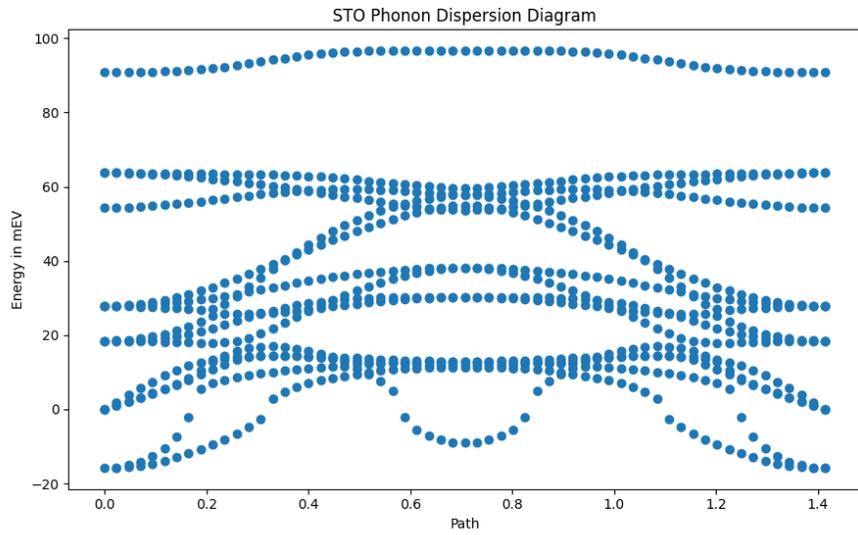


Figure 4.15: DFPT calculated phonon dispersion along  $\Gamma \rightarrow M \rightarrow \Gamma$  – units of meV. Plotted using QE data with Python.

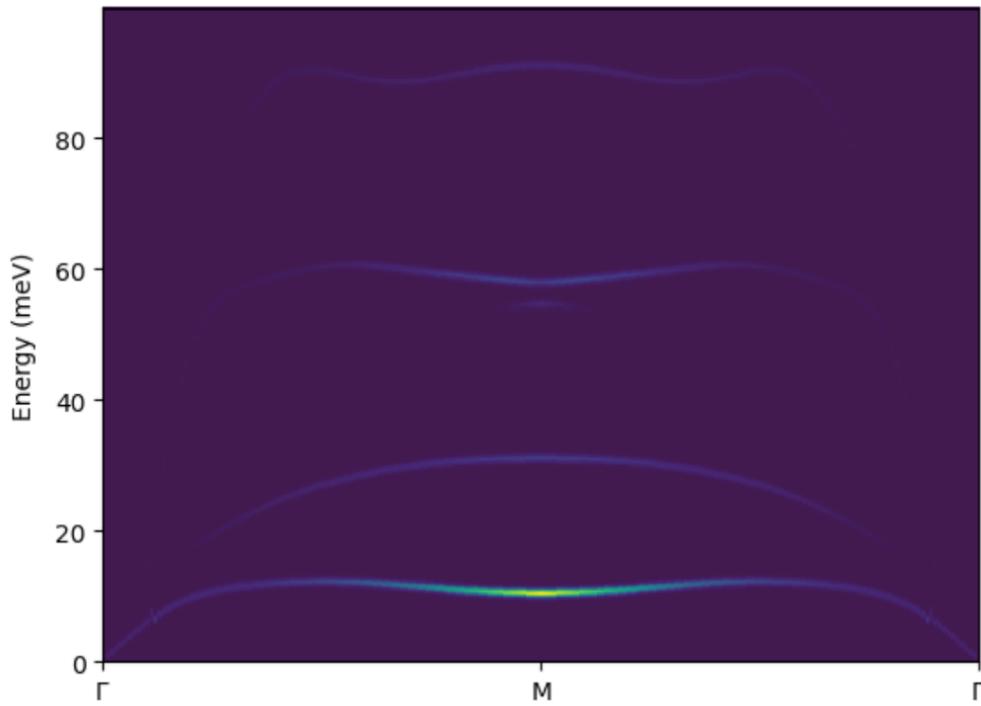


Figure 4.16: Dynamic Structure Factor plot along  $\Gamma \rightarrow M \rightarrow \Gamma$  data produced with Euphonic, plotted with Python. The brighter regions denote higher simulated neutron counts.



Figure 4.17: Dynamic Structure Factor plot along  $\Gamma \rightarrow M$ .

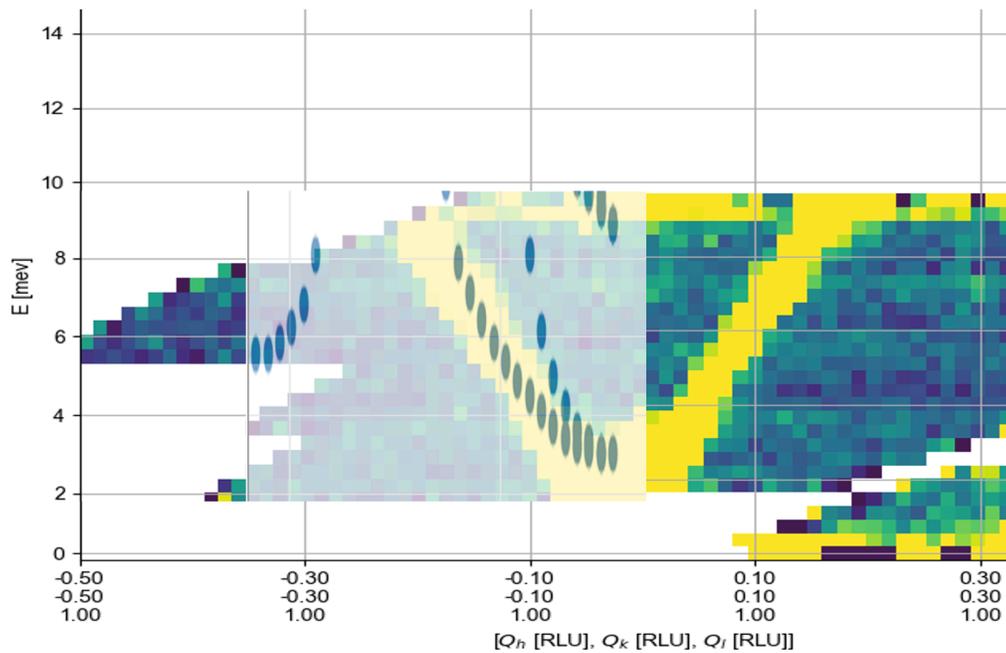


Figure 4.18: DFPT calculated phonon dispersion overlaid with data from CAMEA. We can see good agreement between calculated and experimental results in this particular phonon mode. The Y-axis is again the  $\Gamma \rightarrow M$  path through the BZ.

# Chapter 5

## Conclusions

While we have seen that computational calculations match experimental data in some regimes, the harmonic approximation does not do a satisfactory job describing all phonon properties in this crystalline material.

However, we can conclude that DFT and its derivative, DFPT, are fit for purpose in attributing a suitable initial wavefunction to our STO system, and describing subsequent electronic, thermal and transport properties.

For a better comparison of the two methodologies, improvements can be made on both the computational and the experimental sides. Although in this thesis we used the finite displacement method as well as the DFPT supercell method, there are improvements that can be made: it would be advisable to choose more accurate SCF cycle convergence criteria, increase the number of K-points in the Monkhorst-Pack grid. One can also examine the system using Molecular Dynamics and run calculations on a more capable set of processors.

Experimentally, I propose examining STO using the Merlin Instrument at the ISIS Rutherford Appleton facility in the UK. Using Time-of-Flight spectroscopy, we can achieve much higher energy ranges (8meV - 2000 meV), and neutron intensities up to  $6 * 10^4 n \cdot cm^{-2} \cdot s^{-1}$  [33]. This will provide a much more holistic picture of phonon transport in the material, and subsequently, its thermoelectric properties can be determined.

And finally, it is imperative that work on the Shaking Matters podcast continues. Over the course of the podcast project, it has become even

clearer that outreach activities in the field of materials physics are needed, and are effective since there is already great interest in the final podcast series. As an entry into the genre of science communication, this project has taught me a great deal about communicating complex topics to wide audiences and has also helped cement my understanding of topics in materials physics, and neutron scattering.

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# Appendix A

## Appendix: Shaking Matters Podcast Transcript

Transcripts of the audio recordings have been generated through a combination of manual transcription and the utilisation of OpenAI’s Whisper system [34].

### A.1 Episode 1: Ab initio methods featuring Espen Sagvolden and Edoardo Frititta

00:10.000 → 00:16.720 Hello everyone and welcome to the first episode of Shaking Matters, an investigation into

00:16.720 → 00:25.520 material science and sustainability with me, Shibl Gill. I am currently in Oslo, Norway on a

00:25.520 → 00:32.640 lovely, snowy day, sitting at the offices of Sintef and today I’m joined by Dr. Eduardo Fretitta and Dr. Espen Sagvolden and today we’ll be talking about ab initio methods. We’ll learn

00:40.560 → 00:46.880 a little bit more about what those are in a bit but first I’ll ask my guests to introduce themselves

00:46.880 → 00:51.920 and to tell us a little bit more about their backgrounds. So first I’ll ask Dr. Eduardo.

00:52.880 → 00:58.800 Hi Shibl, thank you so much for having us. Yes, a quick background about introduction about

00:58.800 → 01:06.240 myself. So I am a chemist by training. I have a PhD in theoretical chemistry and ab initio

01:06.240 → 01:12.880 modelings that I obtained from the University of Berlin, the Freie, following to which I

01:13.680 → 01:20.080 did a finished postdoc at King's College London in the same topic with particular focus on

01:20.160 → 01:27.600 strongly correlated materials. Just prior to joining Sinthef in 2021 I also had

01:29.200 → 01:35.360 industrial experience where I learned a bit more about battery materials in particular.

01:35.360 → 01:45.200 That is something that I carried out in my work here at Sinthef. Here I'm dealing with ab initio

01:45.200 → 01:52.400 modeling in a plethora of different projects, one of which is the one we probably would talk

01:52.400 → 01:59.120 about more today, it is the fun projects. There's more focused on again batteries and

01:59.120 → 02:05.520 semiconductors and catalysts and a variety of material of technological interest.

02:06.320 → 02:13.600 Fantastic, thank you. If I may call you Eduardo. Of course. Brilliant and we also have Dr. Espen.

02:14.560 → 02:21.040 Thanks for hosting us. Yes, my name is Espen Saagwilden. I have a PhD in physics

02:22.480 → 02:30.000 focusing on a theory called density functional theory from Tulane University in the United States.

02:33.840 → 02:38.880 After my PhD I did a postdoc in theoretical chemistry

02:39.840 → 02:47.520 and part in in Karlsruhe, Germany and part at UC Irvine in the United States.

02:48.560 → 02:57.440 After which I came here to Sinthef where I'm also like Eduardo working in sort of the

02:59.360 -> 03:06.320 well the area spanning from quantum chemistry to computational solid state physics and

03:06.480 -> 03:12.960 part also on the implementation of quantum chemistry methodology into solid state physics.

03:14.000 -> 03:19.280 Fantastic. Thank you very much to both of you. I recognize that your time is very important and

03:20.960 -> 03:23.600 it's going to be an interesting conversation today.

03:24.880 -> 03:30.320 So first why don't we start with you telling us a little bit more about Sintef.

03:30.640 -> 03:39.680 Yes, so Sintef is one of Europe's largest independent research institutes.

03:40.720 -> 03:48.080 For those familiar with the German institutes it may have most in common with Fraunhofer.

03:49.040 -> 03:59.120 So it is an institute which does both basic science and more industrially related science

03:59.120 -> 04:07.600 for industrial clients. We have about the 1500 scientific employees if I'm not mistaken

04:07.600 -> 04:18.320 of which more than half have PhDs. It covers very wide ranges of science spanning from

04:19.520 -> 04:25.120 the areas where we work which would be more material science, material physics, chemistry,

04:25.280 -> 04:35.040 various technologies towards the green shift I mean fuel cells and photovoltaics and batteries

04:35.040 -> 04:42.160 and so on. Going away from our area we also have an energy department which

04:42.880 -> 04:56.480 focuses more on large energy systems. We have a building institute which

04:56.480 -> 05:07.440 focuses on building science so engineering basically and also an ocean institute which

05:07.520 -> 05:11.120 focuses on marine technologies like fish farming and so. 00:00.000 -> 00:08.240 Thank you very much, Espen. So it seems like Sintef has a number of different arms and

00:08.240 → 00:14.680 is involved in many different disciplines, but the one of greatest interest to me and

00:14.680 → 00:21.120 to our audience is material sciences. And to that regard, Eduardo, why don't you tell

00:21.120 → 00:25.280 us a little bit more about what you're working on in particular?

00:25.400 → 00:32.360 Of course. So as part of, as a research scientist in Sinteph, I'm dealing with a number of

00:32.360 → 00:40.520 projects that require ab initio modeling to describe and predict different properties

00:40.560 → 00:45.200 that can be explained only by taking into account electronic interaction, the electronic

00:45.200 → 00:50.600 nuclear interaction. One of the projects that Espen and I are involved with at the

00:50.600 → 01:01.520 moment is the FUN project. And in this particular activity, our focus is to predict temperature

01:01.520 → 01:07.560 dependent properties of different material of technological interest that you might find,

01:07.560 → 01:16.880 for instance, into semiconductors of solid solid. So in any form of solid state material,

01:17.360 → 01:26.480 it might be ferroelectrics of battery cathodes or anything like that. It is, of course,

01:26.480 → 01:33.600 challenging to get a proper description of those dependencies, because it does require a

01:33.600 → 01:39.880 correct understanding and a correct description of electron-electron interactions, but also

01:39.880 → 01:48.520 electron nuclear and more importantly, nuclear-nuclear interactions and how this change as temperature

01:48.520 → 01:56.240 increase. Also, being the materials of interest being used in different technologies over

01:56.240 → 02:03.080 a quite wide range of temperature, of course, this behavior must be captured in an accurate way. 00:00.000 → 00:09.000 Thank you, Eduardo. So you mentioned ab initio, which often goes along

with ab initio simulations.

00:09.000 → 00:13.000 Now simulations are something which we're all familiar with.

00:13.000 → 00:20.000 But I'm very interested to know what is a simulation to a material scientist?

00:20.000 → 00:28.000 Well, a simulation in general is pretty much trying to find, through computational means in general,

00:28.000 → 00:37.000 a solution to a set of, a very big set, I would say, of simple and yet complex equations

00:37.000 → 00:42.000 that describe all the different, in our case, interactions, but in a more general sense,

00:42.000 → 00:47.000 effects that happen in whatever is your system of interest.

00:47.000 → 00:55.000 Now, in material physics or in material science, of course, those equations describe the nature,

00:55.000 → 01:01.000 describe how, in our case, electrons interact or nucleus interact,

01:01.000 → 01:09.000 but it can describe at a much larger scale how a battery evolves into time

01:09.000 → 01:12.000 once voltage is applied at a specified temperature.

01:12.000 → 01:21.000 So in general, it is basically a study, a simulated, for lack of better words,

01:21.000 → 01:28.000 a study of how a system would evolve given some initial conditions.

01:28.000 → 01:37.000 As you mentioned, the word ab initio means exactly from scratch, from the beginning, from Latin.

01:37.000 → 01:45.000 This is extremely fascinating to us because it's really the concept,

01:45.000 → 01:51.000 the knowledge that we can actually predict accurately some properties of nature

01:51.000 → 01:57.000 by simply considering the rare evidence that comes from experiments

01:57.000 → 02:01.000 and from the natural world of things like electrons behave like waves

02:01.000 → 02:11.000 and electrons are charged particles and yet deliver accurate prediction about the words.

02:11.000 → 02:16.000 This is a fascinating thing and this is exactly what is the building block

02:16.000 → 02:21.000 that leads to then predict things much more complex and much bigger systems.

02:21.000 → 02:32.000 Right, so given some initial conditions and then applying some parameters of how that system evolves,

02:32.000 → 02:37.000 are those principles that can be applied to any system at all?

02:37.000 → 02:42.000 Of course we know about simulations in medicine, in neuroscience,

02:42.000 → 02:47.000 but is there a limit to what can be simulated? Of course, any simulation is only as good as your understanding of the problem and the

00:08.320 → 00:13.440 initial condition that you do provide to your computer code.

00:13.440 → 00:21.000 And it is, as I mentioned, limited by computer resources and by the time that you need.

00:21.000 → 00:31.120 So to the question if anything can be simulated, there is no limit in principle, but there

00:31.120 → 00:38.720 is, of course, some practical limit that is definitely due on how accurate are we actually

00:38.720 → 00:47.360 able to model and to just model the problem at hand.

00:47.360 → 00:52.200 And on the other hand, the computational resources necessary.

So we've mentioned the word *ab initio* now a couple of times, Eduardo what does it

00:06.200 → 00:15.080 actually mean? *Ab initio*. So *ab initio* literally comes from Latin and and the

00:15.080 → 00:20.580 term literally means from the beginning so from first principle and it simply

00:20.580 → 00:25.920 refers to the notion when applied to modeling that we can simulate or predict

00:25.920 → 00:32.320 something simply based on those initial conditions I was talking about that

00:32.320 → 00:39.840 comes straight from first principle straight from some natural and very

00:39.840 → 00:47.040 basic understanding of nature. Example very typical example is in our case of

00:47.040 → 00:52.800 ab initio atomistic modeling the knowledge of electrons are charged they

00:52.800 → 00:59.320 behave like charged particles and they have a specific 1.6 times minus 19

00:59.320 → 01:05.280 coulomb of charge and they do behave like waves and protons have a positive

01:05.280 → 01:10.080 charge opposite to it. I put these three elements together and I'm able to predict

01:10.080 → 01:16.160 the atomic level of the hydrogen atom. This is the the most basic definition of

01:16.160 → 01:20.360 ab initio I can give. Building on top of that comes the whole field that arrives

01:20.440 → 01:29.480 to predict structure of very complex crystals or or enzymes or anything you

01:29.480 → 01:34.400 can imagine it is based on chemistry. So currently what are you able to

01:34.400 → 01:41.440 simulate using just purely ab initio methods given given the accuracy that

01:41.440 → 01:46.760 they provide so what kinds of systems have you been able to model quite

01:46.800 → 01:54.000 effectively? So the limit is definitely given by size and complexity and by the

01:54.000 -> 01:59.600 computer power that is available and I would say that at the state of the art

01:59.600 -> 02:06.560 we find ourselves in small or medium sized molecules for instance can be

02:06.560 -> 02:12.120 routinely done with arbitrary accuracy. However as we start moving into

02:12.160 -> 02:17.280 territories or more larger even biomolecules so we get into periodic

02:17.280 -> 02:22.760 systems for instance the ones of interest we mentioned a few times like

02:22.760 -> 02:30.600 batteries or for electrics or things like that that do contain atoms with

02:30.600 -> 02:36.280 several electrons and very complex electronic-electronic interaction

02:36.280 -> 02:39.840 effects then the situation starts become much more challenging and we start

02:39.840 -> 02:46.800 really hitting a wall. So I would say yeah I would say nothing. So, it sounds like we're in the regime of the very, very small, perhaps even in the quantum

00:07.280 -> 00:08.280 regime.

00:08.280 -> 00:13.560 So, in these systems that Eduardo is talking about, atoms and molecules, when we talk about

00:13.560 -> 00:19.280 simulating those systems, what exactly are we looking to find?

00:19.280 -> 00:28.480 Yeah, what we are looking to find is, of course, the values of certain physical properties,

00:28.480 -> 00:32.320 quantities, known as observables.

00:32.320 -> 00:40.840 But what we, in practice, are computing is a quantity known as the wave function.

00:40.840 -> 00:47.680 Because I mean, when you get down to the scale of electrons, atoms, molecules, I mean, many

00:47.680 -> 00:57.380 of the computations we're doing are on the scale of a couple of cube non-meters or something

00:57.380 → 01:06.620 like that, then Newtonian mechanics, as most of us know it, no longer apply, especially

01:06.620 → 01:08.540 not to the electrons.

01:08.540 → 01:12.780 There are completely different rules of nature applying.

01:12.780 → 01:23.100 The wave functions and also the nuclei, by the way, are expressed or behave more as waves

01:23.100 → 01:27.140 in a mathematical object known as the wave function.

01:27.900 → 01:36.940 The behavior of the wave function, both the states it can be in, which in many cases are

01:36.940 → 01:39.540 discrete states.

01:39.540 → 01:48.740 And also its time evolution are governed by something called the Schrodinger equation.

01:49.140 → 02:03.260 This finding the wave function based on this Schrodinger equation is really a very multidimensional

02:03.260 → 02:05.020 mathematical problem.

So, Espen, myself included, I think many of us have seen the Schrodinger equation and

00:07.640 → 00:13.120 we might even have worked with it a little to some extent, so why is it so difficult

00:13.120 → 00:19.800 to solve given that it fits quite nicely on one line, and why is it so important for us

00:19.800 → 00:24.240 to solve this equation in order to do our simulations?

00:24.560 → 00:31.600 Yes, solving the Schrodinger equation for one particle is easy. I mean, that's like

00:31.600 → 00:39.600 undergraduate textbook stuff with the hydrogen atom and so on. What lends complexity to the

00:39.600 → 00:46.840 problem is the electron-electron interaction term. Without the electron-electron interaction

00:46.840 → 00:54.480 term, you could actually express the wave function as one quite simple mathematical object.

00:54.480 -> 01:03.480 That, however, becomes impossible once the electrons start repulsing each other, in which

01:03.480 -> 01:13.880 case you really, in today's methods, have to express the wave function with a very high

01:14.200 -> 01:21.400 mathematical degree of complexity in order to really account for the ways in which electrons

01:21.400 -> 01:30.920 avoid each other. And this is very important because it is only when you see the electron-electron

01:30.920 -> 01:42.600 avoidance in the wave function, that's sort of what gives many of the physical properties

01:42.600 -> 01:51.760 of the actual system. I mean, in the sense that it gives the energies and implicitly

01:51.760 -> 01:53.600 also many of the other observables. So we've talked about doing these simulations on big enormous computers, but why don't

00:08.800 -> 00:20.960 we just go to an instrument or a lab and run our experiments there and try and model how

00:20.960 -> 00:27.160 a system is going to evolve and get it directly from an experimental apparatus?

00:28.120 -> 00:34.440 Well, to answer this I would look at what actually models are doing for us.

00:36.280 -> 00:43.720 To me, the answer is threefold. On one side, it's computer models, an issue or not an issue that

00:43.720 -> 00:49.560 they are. Do the exact same thing that we've always been doing since the beginning of science,

00:49.560 -> 00:56.280 when time to interpret data. If you have a set of experimental data that you need to

00:57.080 -> 01:03.560 understand and make sense of, in general you fit those data or try to interpret those data

01:03.560 -> 01:09.880 through some physical law or through some linear or non-linear fit that comes from

01:10.680 -> 01:19.320 a simple or complex understanding of reality. What we do here is just a build up on top of that.

01:19.960 → 01:28.600 So now our equations are more complex than a very simple or compact linear or exponential form

01:28.600 → 01:35.080 that it might be. They actually do require not to, they cannot be expressed as a simple equation

01:35.080 → 01:40.680 or a simple trend, but they do require to be in data form, data form that comes from the model

01:40.680 → 01:46.760 in itself. But in my mind it is the exact same thing. You still construct this model that is now

01:46.760 → 01:53.400 a bit more complex to interpret experimental data. On the other hand, a second importance of

01:53.400 → 01:59.720 performing modeling is that it actually allows you to do things that you couldn't do experimentally.

01:59.720 → 02:07.640 There are a number of properties that you can indirectly gather, but not directly measure,

02:07.640 → 02:13.400 while through a initial modeling you can really create this lens provided, of course,

02:13.400 → 02:19.240 that your model is accurate, but you can really have this lens over the quantum and over the

02:19.240 → 02:24.840 atomistic world and really get the number and the properties that you wanted without too much

02:24.840 → 02:31.320 hassle. And actually sometimes you actually can't. And the first thing is cost and time.

02:31.960 → 02:39.240 Often experiments are extremely costly and extremely time consuming. And especially when

02:39.320 → 02:46.040 the question that is given to us is find a new, better material for a special application.

02:46.600 → 02:53.880 Now scanning, as we say, or trying and testing a bunch of different materials experimentally,

02:53.880 → 03:02.040 it starts becoming prohibitive, where it is much more easily achievable through what we call

03:02.040 → 03:11.800 high throughput scanning of material through computation. To me, the importance of modeling

03:11.800 → 03:20.280 really comes from these three things together. This, of course, doesn't take away the fact

03:20.280 → 03:27.320 that some people sustain that experiments are still going to be carried out and they're still

03:27.320 → 03:32.840 the cornerstone of scientific, scientific development. We do need experiments because

03:32.840 → 03:41.000 those are really the truth. The experimental data is really how reality and how the natural world

03:41.000 → 03:47.320 is actually behaving. But this support and this guideline given by this sort of digital team,

03:47.320 → 03:52.520 twin if you want, are key for actually pushing the boundary as possible.

03:52.520 → 04:00.120 So it sounds like having the ability to model these systems on a computer or on a very powerful

04:00.120 → 04:09.480 computer is a very important piece of kit in the armor of material science. It allows you to do

04:09.480 → 04:18.040 science which would otherwise be very difficult to do or out of reach or in some cases even impossible. eah, so if I can add on what, or elaborate on what Eduardo has already said, I think,

00:08.400 → 00:16.460 so for instance, when it comes to using theory in, as a model, so to speak, for interpreting

00:16.460 → 00:25.240 experiments, I mean, you can see this in spectroscopies, for instance, I mean, people run IR spectroscopy

00:25.480 → 00:34.520 or UV visual spectroscopy, they get out the spectrum, but then it has become customary to

00:34.520 → 00:42.040 then run a computation, a quantum chemistry computation, in order to assign sort of, okay,

00:42.040 → 00:50.440 so this peak is this vibration and that peak is that vibration. The results, so I think

00:51.160 → 00:59.480 the element that some stuff, I mean, if you want, you don't want it in your lab, you don't want

01:00.040 → 01:10.440 material from nuclear reactors, for instance, in your microscope, but it's completely fine to run

01:10.680 → 01:21.160 theoretically. One further aspect of theoretical computations is that you can actually do counterfactual

01:21.160 → 01:30.360 things. I mean, like, you can't, maybe in nature, you won't find this surface because it's too reactive,

01:30.360 → 01:37.960 you won't find atoms going into some area because they, it's energetically unfavorable, but when

01:37.960 → 01:45.240 running a computation where you can dictate the chemical environment, dictate the position

01:45.240 → 01:52.040 of the various atoms, you can actually simulate that case. So it seems to me that in order to be able to do good computer simulations of these systems

00:08.800 → 00:16.840 in physics or chemistry, it requires a number of very complex physics problems to be solved.

00:16.840 → 00:26.480 So can you give us a brief history of trying to model these systems computationally and

00:26.480 → 00:28.720 in what areas they've been useful?

00:29.440 → 00:41.520 Yes, so you can say the earlier methods within the area, those are methods where the electrons

00:41.520 → 00:49.600 are basically described as interacting with the other electrons only in an average way.

00:49.600 → 00:54.720 They feel some sort of average potential, average interaction with the other electrons.

00:54.720 → 01:01.840 So then you avoid this problem that we spoke about earlier that it's the electron-electron

01:01.840 → 01:10.800 interaction which messes up the entire solution of the Schrodinger equation and you get a relatively

01:10.800 → 01:18.560 simple solution of the problem. Of course, this approximation can only be so good sort of

01:19.520 → 01:28.080 in that it doesn't explicitly take into account most of this electron-electron avoidance.

01:29.120 → 01:39.120 So then going past that you could say that the history of computational quantum chemistry or

01:40.080 -> 01:49.040 especially branches into two directions. One is adding complexity to the wave function

01:49.840 -> 01:57.360 so that it to a larger and larger extent actually explicitly expresses how the two

01:57.360 -> 02:07.760 electrons or many electrons avoid each other. The other is this area known as density functional

02:07.760 -> 02:14.080 theory where what you compute is actually even simpler than the wave function, simply the

02:16.000 -> 02:20.960 average particle density, the electron density and its spatial distribution.

02:21.520 -> 02:28.720 But then you can, well there are different approaches in DFT but you can say that some

02:28.720 -> 02:36.320 of the physically more grounded approaches may in some cases involve that you superimpose a model

02:36.320 -> 02:45.600 of how electrons avoid each other onto this density. So both these wave function methods that I

02:45.600 -> 02:52.560 mentioned in the start and DFT are used in quantum chemistry whereas in computational solid state

02:52.560 -> 02:56.880 physics it's mostly DFT which is being used. o, there is a plethora of methods, there is really a zoo of methods, and in many cases

00:10.480 -> 00:15.120 it has happened, as the kind of aspen was mentioning, there's been a natural historic

00:15.120 -> 00:20.800 evolution from less accurate to more accurate, but it's in nowadays is not necessarily the

00:20.800 -> 00:21.800 case.

00:21.800 -> 00:28.440 Oftentimes we do prefer to use one method or another depending which kind of system we

00:28.440 -> 00:29.440 are describing.

00:29.840 -> 00:37.800 If I am interested in describing a molecular system, I'm not going to apply the same methodology

00:37.800 -> 00:45.440 that I would if I have, say, a solid state system with strongly correlated transition

00:45.440 → 00:50.480 metal, and it's the same, I wouldn't apply the same system that I use for a periodic

00:50.480 → 00:54.360 solid system that doesn't contain the strongly correlated material, the strongly correlated

00:54.360 → 00:55.360 sites.

00:55.360 → 01:03.560 So, there is often times there is a tool for the problem at hand, and it's true that those

01:03.560 → 01:08.480 tools are evolving over time and are improving over time, but there is always a, we really

01:08.480 → 01:13.280 have a arsenal at our disposals, and depending what we need to do, we'll make a choice of

01:13.280 → 01:14.320 exactly what to use. o if you were to be able to find the full description of the wave function, would it

00:08.000 → 00:13.000 be fair to say that then you can describe the whole solid?

00:13.000 → 00:24.000 No, because you can say that when we do computations in solid state physics, what we assume is that

00:24.000 → 00:34.000 we have many, many small identical building blocks that repeat infinitely in all three spatial directions.

00:34.000 → 00:39.000 So you're basically assuming a perfect crystal.

00:39.000 → 00:48.000 And that's not the way nature is. I mean, you have all sorts of defects in a crystal.

00:48.000 → 00:57.000 It might be impurities, it might be grain boundaries, it might be anything.

00:57.000 → 01:09.000 And many physical properties such as say electrical conductivity, thermal conductivity, which is the theme of the fund project, for instance.

01:09.000 → 01:33.000 I mean, they are multi-scale phenomena and also these higher size scale effects will have profound influence on these physical observables that we cannot model within our approach. o, that sort of begs the question. So far, and in a typical case, how to have an issue

00:11.560 -> 00:18.680 computational methods compared with experimental data that's been gathered? And if there's

00:18.680 -> 00:22.320 a gap, how wide is the gap?

00:22.320 -> 00:29.600 As often with this kind of question, the answer is it depends. And it really does depend

00:29.600 -> 00:38.380 mostly on the scale of interest of your phenomena that you're trying to describe and of the

00:38.380 -> 00:45.200 size of the system itself that you're trying to model. If your question is, for instance,

00:45.200 -> 00:53.640 what is, can you model the energy levels of an atom or a small molecule, so the electronic

00:53.640 -> 00:59.120 energy levels or even vibrational levels? I would tell you with confidence that we

00:59.120 -> 01:05.680 are very, very, very close to the exact answer, almost hitting the exact answer with arbitrary

01:05.680 -> 01:14.440 accuracy. If now your system of interest is becoming something much larger, and as it

01:14.440 -> 01:19.680 was mentioned at some point, you start having, for instance, imperfections. Say it's a solid

01:19.680 -> 01:24.680 and you start having imperfections. And the presence of those imperfections has effect

01:24.720 -> 01:30.480 on the final property you're trying to measure. Or say something a bit more complex. Say you

01:30.480 -> 01:40.400 want to get catalytic activity, for instance, of a surface. And this is not a clean cut surface,

01:40.400 -> 01:46.240 but for instance, it's something very rough that contains a lot of imperfections and it's

01:46.320 -> 01:53.760 very heterogeneous materials. Now, being able to capture all of the different

01:55.360 -> 02:02.640 pathways that a reaction could have on such complex systems, it's nearly impossible for

02:02.640 -> 02:14.280 modeling. We can get the main trend, perhaps. But again, it really depends on what are you

02:14.320 → 02:21.560 trying to model. Now, statistical or a thermodynamic leverage is, I would say, you can pretty much

02:21.560 → 02:32.280 get with confidence. But it's a very wide subject. But anyway, so this is kind of to say

02:32.280 → 02:43.560 that fundamental principles, so actually properties that depends on fundamental principles are

02:43.560 → 02:52.360 fairly accurately described. Properties that depends on the specifics of the micro or

02:52.360 → 03:01.640 macro scale details of my materials. Those, of course, are through a miniature modeling out of

03:01.640 → 03:09.320 reach at the moment. Right. But that is not to say that more work in the field cannot help

03:09.400 → 03:19.800 close the gap. No, absolutely not. It is, of course, there are, of course, two major directions

03:19.800 → 03:25.880 that the field constantly moves and rides along to. One being the computational power that is

03:25.880 → 03:33.160 constantly increasing, something like doubling or quadrupling every single year. And the other is

03:33.160 → 03:39.880 the development of more efficient and yet more accurate methodologies. These two things, of

03:39.880 → 03:48.760 course, go hand by hand. And the systems that we can model today were a dream or impossibility

03:49.320 → 03:56.040 a few years ago. And what we cannot model today, it will be routine in a few years. This is

03:56.040 → 04:04.440 constantly ongoing all over all fields of material modeling. So there definitely will be

04:04.440 → 04:12.520 a point where we'll be able to model something that now I would say, yeah, maybe let's avoid that. And how is the fund project that you're both involved in, how is that helping to close this gap?

00:08.000 → 00:16.000 So, so far in our discussion we have been talking a lot about the electronic problem, how electrons

00:16.000 → 00:22.000 interact and how this whole electronic wave function can or cannot be obtained.

00:22.000 → 00:29.000 But in the fund project we are interested in to getting out a proper description of the

00:29.000 → 00:34.000 thermal dependencies of key properties of materials.

00:34.000 → 00:40.000 And in order to get that you need to not only have a proper description of electronic interaction

00:40.000 → 00:44.000 but also to have a proper description of the nuclear wave function itself.

00:44.000 → 00:53.000 And what we will do is that we will use some new techniques that have been developed in the field

00:53.000 → 01:01.000 that move beyond what is currently available in standard ab initio codes, mostly based on

01:01.000 → 01:07.000 perturbation theory, and couple those with very fine-tuned neutral scattering experiments

01:07.000 → 01:16.000 to really push forward the understanding, not only the understanding of this physical phenomena

01:16.000 → 01:25.000 but actually get a computational platform that can allow us to predict new materials that have not been discovered yet.

01:25.000 → 01:32.000 Right, so it seems like you have a computational arm in this fund project and an experimental arm

01:32.000 → 01:39.000 and then in the middle you try and meet and reconcile the differences in the data

01:39.000 → 01:46.000 and try to apply statistical methods to have a better understanding of where the shortcomings are

01:46.000 → 01:50.000 in the computational model and where it can be improved.

01:50.000 → 01:52.000 You can say that. Yes, you can say in many ways, so from our side, what we're doing, as Eduardo said, we're

00:13.360 → 00:22.640 using new methodologies and it's important for us to have those verified by experiment.

00:22.640 -> 00:35.640 This is typical within the area of computational, well both chemistry and solid-state physics.

00:35.640 -> 00:47.680 In the end, the natural sciences are empirical sciences and if a theory cannot reproduce nature,

00:47.680 -> 00:51.880 then something is wrong in the theory.

00:51.880 -> 01:08.080 Also here, it's crucial for us to have a good experimental verification of those phenomena.

01:08.080 -> 01:16.840 In our case, heat transfer or heat transport phenomena that we are trying to model.

01:16.840 -> 01:28.840 So, in having that experimental verification would give us confidence to apply these models also to other systems later on.

01:28.840 -> 01:39.840 Right, so once you are able to close this gap between computational modeling and experimental physics,

01:39.840 -> 01:43.840 what are the advantages that you foresee for the industry?

01:43.840 -> 01:55.840 Does it mean that you might be able to model more and more complex systems computationally, perhaps be able to discover more materials?

01:55.840 -> 01:58.840 What could you say on that?

01:58.840 -> 02:10.840 Absolutely, I mean, if you can have confidence in your theoretical model, that also means that you can go on larger computational campaigns.

02:10.840 -> 02:27.840 But I think it sort of goes a little bit beyond that also in that once you gain theoretical insight, for instance, in the relative importance of various physical phenomena,

02:27.840 -> 02:39.840 that also gives you, well, so to speak, the intuition to know in which direction to move when you try to improve something.

02:39.840 -> 02:51.840 The investment that has been made in the past few decades into digitalization, not only into the academic sector, but more importantly into the industrial sector is extremely massive.

02:51.840 -> 03:01.840 And this should have something to say about

the importance of the role that experts like us are playing into the development of new materials,

03:01.840 → 03:15.840 that have a wide range of applications, of course, ranging from electronics all the way down to energy storage, energy production,

03:15.840 → 03:21.840 and development of, okay, I lost myself. 00:00.000 → 00:06.440 The huge investment that has been done in the past few decades, not only in academia but

00:06.440 → 00:15.120 especially into industry, into digitalization and computational tools, it's really telling

00:15.120 → 00:23.160 about the power of those approaches into really pushing forward the industry and material

00:23.160 → 00:26.480 development and material discovery.

00:26.480 → 00:33.920 And this ranges all over the spectrum of natural sciences and all over the spectrum

00:33.920 → 00:44.000 of, for instance, new renewable energies, whether it is for energy storage or whether

00:44.000 → 00:53.120 it is for energy production, whether we're dealing with finding new, for instance, photovoltaic

00:53.120 → 01:02.560 materials with higher efficiencies or batteries that can deliver with higher power and can

01:02.560 → 01:10.960 have higher energy densities and can have higher fast charging or whether it is for

01:10.960 → 01:19.440 describing a catalyst that can help with carbon capture or finding new cleaner fuels.

01:20.400 → 01:27.280 These are all aspects that, in a way or another, are covered not only at SINTEF but in general in the

01:27.280 → 01:37.680 overall industrial and academic arena these days, not experimentally and particularly in modeling.

01:37.680 → 01:43.440 Right, so the work that you're doing, it's touching not just material physics but a whole

01:43.520 → 01:50.400 number of fields and in particular it's helping material physics come onto the front line of

01:50.400 → 01:57.600 fighting this climate crisis that the world is facing. So it seems more important than ever

01:58.800 → 02:05.840 that this work is supported and that people become more interested in it and governments

02:05.840 → 02:09.120 continue to support your work.

and you can say science, I mean both experimental science and computational science on questions

00:10.240 → 00:16.600 having to do with the green shift are much wider than what you could, I mean, typically

00:16.600 → 00:24.320 imagine you would imagine that, okay, you're faced with a battery, you simulate the batteries

00:24.320 → 00:31.320 function, for instance, same with a photovoltaic and so on. And that's one thing, but there

00:31.320 → 00:38.520 are so many other questions surrounding many of these technologies that you don't immediately

00:38.520 → 00:47.920 think of. So for instance, I'm involved in a project where we're computing ice formation

00:47.920 → 00:53.720 on windmills. So I mean, it doesn't go directly to the function of the windmill, but it's

00:53.720 → 00:57.400 still a societal problem if you have ice formation on the wings. So it's becoming more apparent that there are a number of arenas where successes in material science are helping us in this fight against the climate crisis.

00:14.000 → 00:22.000 Another thing I've been very curious about, about your work here at Sintep, it seems like, well at least in the past,

00:23.000 → 00:32.000 physicists would generally associate only with other physicists and same with researchers in other fields.

00:32.000 → 00:36.000 They tend to remain within their silos.

00:36.000 → 00:45.000 But it seems like at Sintep you have a renewed focus on a multidisciplinary approach to your problem solving.

00:45.000 → 00:59.000 Do you have any insights on that or any examples of situations where you've worked with colleagues from across the aisle, so to speak, to achieve better outcomes?

00:59.000 → 01:07.000 Absolutely. This is something that is, as you mentioned, extremely encouraged at Sintep and for good reasons.

01:07.000 → 01:18.000 Because we have an ever-growing number of experts in almost any field of natural science that you can imagine.

01:18.000 → 01:33.000 Collaborations with, for instance, Sintep Digital for the development of new codes or new AI platforms, ontologies, this is very much ongoing.

01:33.000 → 01:49.000 In our own niche as ab initio modelers, of course the support we can provide doesn't limit itself to, say, solid-state physics materials.

01:49.000 → 01:57.000 But we can also stand anywhere, really, where you have a problem that involves atom and molecules. And finally, gentlemen, something I've been interested in for a while is taking on a multidisciplinary approach to problem solving.

00:10.000 → 00:24.000 Now, since I've been here at SYNTF, I've noticed that there's quite a bit of focus on adopting a collaborative, multidisciplinary approach to problem solving.

00:25.000 → 00:34.000 Would you like to speak about the benefits of such an approach and perhaps if you've encountered it within your work?

00:34.000 → 00:43.000 Sure. So SYNTF is really a unique place to work in. I've been here for a bit more than a year, perhaps.

00:44.000 → 00:52.000 And yet, I can say that compared to any other place I've ever worked in, you have this industrial focus.

00:52.000 → 01:01.000 All our activities, of course, verge towards eventually development of technologies for the industry benefit.

01:01.000 → 01:15.000 And at the same time, you have this academic imprint, in a way, that is the interest, of course, of the main research scientist of understanding nature.

01:15.000 → 01:28.000 And because of the nature of all different industrial problems that we need to solve, the stuff, it's extremely varied in competencies.

01:28.000 → 01:38.000 And pretty much whatever problem you have, if you don't know something, you can be sure that there is somebody else

in the institution who has the answer for you.

01:38.000 → 01:49.000 Multidisciplinary or interdepartmental or interinstitutional collaboration and activities are strongly encouraged here.

01:49.000 → 01:51.000 And there are highly beneficial.

01:51.000 → 02:00.000 Those are definitely the best projects we can have are the ones where we actually put together our brains and we find the solutions together and it shows.

02:00.000 → 02:06.000 Both in terms of actually finding a solution for whether it is an academic or industrial problem that it is.

02:06.000 → 02:17.000 Both of it is to actually construct a very strong consortium for submitting applications for public fundings.

02:17.000 → 02:28.000 So yes, this is definitely something that is happening here and it's extremely exciting to work in this environment.

02:28.000 → 02:40.000 Fantastic. Well, gentlemen, thank you very much for your time. It's been a very enlightening conversation and we wish you all the best in your work in the future.

02:40.000 → 02:42.000 Thank you so much for having us.

## **A.2 Episode 2: ISIS Instrument Scientists**

### **A.2.1 Dr. Duc Lee**

Right, now I have with me Dr. Duc Lee, an instrument scientist here at ISIS.

00:08.000 → 00:16.000 Dr. Lee, why don't you introduce yourself and tell us a little bit about your journey so far at ISIS?

00:16.000 → 00:22.000 Hi, I'm Duc Lee, an instrument scientist at the ISIS Neutron and Muon source.

00:22.000 → 00:32.000 I'm responsible for a time-of-flight spectrometer called MARI, which is used to measure the excitations in materials,

00:32.000 → 00:38.000 so essentially how atoms move and where they are, essentially as well.

00:38.000 → 00:44.000 I've been at ISIS seven years now, so it's been a while.

00:44.000 → 00:55.000 I did my PhD at UCL. I then went and did a postdoc in Berlin and then another postdoc in Korea,

00:55.000 → 01:04.000 both on neutron-related studies. I was into studying magnetism at the time, magnetism of rare earth materials.

01:05.000 → 01:15.000 Since then, I've, I guess, moved a bit more into functional materials and also computing,

01:15.000 → 01:22.000 so my current project is to use machine learning for data analysis.

01:22.000 → 01:29.000 Yeah, so I don't know if you want to go into any of those in detail yet.

01:29.000 → 01:35.000 That's fantastic. So we've spoken with a few instrument scientists here at ISIS,

01:35.000 → 01:43.000 but I'm really interested to know what your day-to-day work looks like and whether you get the chance to pursue your own research

01:43.000 → 01:51.000 or work with users or help with upgrades at the instrument and so on.

01:52.000 → 02:00.000 It's quite varied, so we run for, the accelerator runs for about half a year, 150 days-ish,

02:00.000 → 02:08.000 so when we're running and when we're doing experiments then I would be on the instrument a lot,

02:08.000 → 02:16.000 working with users, helping them with their experiments, taking data, doing some data analysis, that kind of thing.

02:16.000 → 02:22.000 On the other hand, when we're not running, I'm usually just in the office, on the computer,

02:22.000 → 02:31.000 doing more data analysis or debugging programs or writing papers, that kind of thing.

02:31.000 → 02:34.000 Sounds like there's many different components to your job.

02:34.000 → 02:35.000 It's quite varied, yeah.

02:35.000 -> 02:41.000 So I wonder which parts of it are most appealing to you and most interesting,

02:41.000 -> 02:47.000 and I'd also like to know how that's changed over the course of your scientific career.

02:47.000 -> 02:53.000 So I think the best part is probably doing the experiments.

02:53.000 -> 02:55.000 That's usually the most fun.

02:55.000 -> 02:59.000 So it's hands-on, it's practical.

02:59.000 -> 03:04.000 You also meet a lot of people, like the users come from all around the world.

03:04.000 -> 03:08.000 We get a lot of people from India, from across Europe,

03:08.000 -> 03:12.000 so a few from the US, but not so many.

03:12.000 -> 03:17.000 And it's always fun to chat and discuss what they're doing

03:17.000 -> 03:23.000 because there sometimes can be quite different science to me, and sometimes very interesting.

03:23.000 -> 03:27.000 Especially that I've branched out into more functional materials

03:27.000 -> 03:30.000 because a lot of the users we get on Mari are chemists

03:30.000 -> 03:36.000 who are making, say, alternative lithium ion battery cathode materials

03:36.000 -> 03:39.000 or ionic conductors or something like that.

03:39.000 -> 03:44.000 And I had no background in this before, so it was picked up from users.

03:44.000 -> 03:48.000 So yeah, it can foster some collaborations, and if you get on well with them then, yeah.

03:48.000 -> 03:50.000 It's really nice, yeah.

03:50.000 -> 03:55.000 So that's probably the most fun part of the job.

03:55.000 -> 03:59.000 But on the other hand, we don't run that much

03:59.000 → 04:07.000 because being a party accelerator costs a lot of, in electricity, costs to run the facility.

04:07.000 → 04:13.000 So we don't run as much as we would like, essentially.

04:13.000 → 04:21.000 Overall, how do you visualise the work that you do on a day-to-day basis

04:21.000 → 04:28.000 affecting the bigger picture of where experimental physics is

04:28.000 → 04:34.000 and where computational physics and materials physics.

04:34.000 → 04:39.000 So how does your work and the work of Pisces in general

04:39.000 → 04:45.000 fit into the larger picture of pushing the other guard of science forward?

04:45.000 → 04:48.000 Well, that's it.

04:48.000 → 04:53.000 I mean, I think a lot of modern science research is,

04:53.000 → 04:59.000 you just tend to be quite a small cog in a very big machine and so forth.

04:59.000 → 05:04.000 So I guess it's more incremental.

05:04.000 → 05:09.000 So there are different types of users.

05:09.000 → 05:17.000 So on the functional material side, on the batteries, the thermal electrics,

05:17.000 → 05:21.000 we get people who are synthesising new materials

05:21.000 → 05:37.000 and then they just come to us to characterise it, to work out why certain materials conduct heat in such a way.

05:37.000 → 05:42.000 And some of the measurements will give you hints.

05:42.000 → 05:46.000 I mean, it doesn't always give you complete answers, but it will give you hints

05:46.000 → 05:50.000 if you do something else.

05:50.000 → 05:52.000 So it's all little bits, I guess.

05:52.000 → 05:56.000 It helps contribute to a bigger picture, but it doesn't.

05:56.000 → 06:04.000 I'm not sure there's many techniques that would tell you exactly everything that's going on with all the atoms by itself.

06:04.000 → 06:11.000 So the inelastic neutron scattering, which is what I do, will give you some extra detail.

06:11.000 → 06:19.000 So for example, if you've got a thermal electric, you tend to want them to be bad heat conductors.

06:19.000 → 06:25.000 So you want them to be quite good insulators so that you maintain a temperature gradient.

06:25.000 → 06:31.000 So you generate electricity by having a temperature gradient, which causes a voltage gradient.

06:31.000 → 06:39.000 But you don't want the hot and cold sides to equalise.

06:39.000 → 06:42.000 So you want something that's a bad conductor.

06:42.000 → 06:52.000 And we know a lot about how materials conduct heat.

06:52.000 → 07:02.000 And it's to do a lot with how they move, and that's what you can measure with an inelastic neutron scattering.

07:02.000 → 07:13.000 But it's a bit of an indirect method, so you also need to do calculations in order to say for sure that this is how they move,

07:13.000 → 07:18.000 and this is why they don't conduct heat, for example.

07:18.000 → 07:31.000 So from your vantage point, what advancements or near research are you most excited about in the field?

07:31.000 → 07:33.000 Any highlights for you?

07:33.000 → 07:44.000 So I mentioned before, I think I move fields every three or four years because I've got a short attention span.

07:44.000 → 07:49.000 So the thing I'm most enthusiastic about right now is machine learning.

07:49.000 -> 07:57.000 So it's been in the news a lot, partly because of the hardware we've got now.

07:57.000 -> 08:05.000 So we can just run some models that would help us in our data analysis on some of the servers that we've got,

08:05.000 -> 08:11.000 or possibly on a standard desktop with a good graphics card.

08:12.000 -> 08:24.000 But yeah, so now instead of having a big facility, some large cluster, you can actually run something individually.

08:24.000 -> 08:33.000 And furthermore, there's a lot of the software libraries available, so it's a lot easier to apply machine learning techniques to diverse fields

08:33.000 -> 08:40.000 that's not about selling you things, advertising or things like that.

08:40.000 -> 08:52.000 So yeah, I'm really interested in applying this to speed up our data analysis because in some cases it takes months or years,

08:52.000 -> 09:02.000 so often we would get scientists who come in and they would have a PhD student,

09:02.000 -> 09:09.000 and you've got one PhD student, one project, and it would take them two or three years to analyze the data.

09:09.000 -> 09:15.000 It just takes a long time, but maybe we can get machine learning to speed it up.

09:19.000 -> 09:30.000 So finally, for the students and the non-traditional students out there who might want to get involved in the cutting edge of science today,

09:30.000 -> 09:36.000 what advice would you have and how would you counsel them?

09:39.000 -> 09:47.000 I think you have to be really almost obsessive. I don't know if I would counsel that,

09:47.000 -> 09:57.000 but you don't have to be the smartest person. You do kind of have to be a bit obsessive, I think.

09:57.000 -> 10:00.000 But I don't know where that's at.

10:00.000 -> 10:07.000 But within that, there is the option for students to pick their specialization,

10:07.000 -> 10:15.000 and it's not necessary that they stick with whatever they did in their master thesis.

10:15.000 -> 10:19.000 No, no, but I think you have to pick something that you enjoy.

10:19.000 -> 10:26.000 So I mean, don't pick something because you think it will make you famous or something.

10:27.000 -> 10:34.000 It will be a lot of work, and if you don't enjoy it, then you probably won't stick with it.

10:34.000 -> 10:41.000 And within science, really, we know that it's almost impossible to predict what will be the next big thing,

10:41.000 -> 10:45.000 and the next field of research that's going to capture everyone's attention.

10:46.000 -> 10:51.000 So, yeah, I think you don't have to... I mean, what you pick when you start your PhD

10:51.000 -> 10:56.000 is not necessarily what you'll be doing even five years down the road afterwards.

10:58.000 -> 11:02.000 Yeah, so a lot of the skills that you learn will be transferable,

11:02.000 -> 11:11.000 so that the analytical skills and nowadays computer programming is a big part of it as well.

11:12.000 -> 11:17.000 Yeah, whatever you research that will carry over.

11:17.000 -> 11:22.000 So, yeah, I think just pick something that you really like.

11:22.000 -> 11:25.000 Well, that's great advice for anyone.

11:25.000 -> 11:27.000 Thank you so much, Dr. Dickey.

11:27.000 -> 11:32.000 Thank you for your time. We appreciate your wise words.

## A.2.2 Dr. Gjørn Nielsen

So I'm responsible for polarized neutrons here at ISIS. So what is a polarized

00:05.400 → 00:10.920 neutron? Well actually we're talking here about polarized neutron beams. So

00:10.920 → 00:17.240 neutrons have a spin of one half and that means that in external magnetic field

00:17.240 → 00:21.440 they can point either along that field or opposite to it. So we call these the

00:21.440 → 00:26.160 up and down states of the neutrons. And a polarized beam is one where you have

00:26.160 → 00:32.000 predominantly the up or the down state in the beam. So why do we prepare these

00:32.000 → 00:36.400 polarized beams? Well it turns out that using polarized beams can tell us more

00:36.400 → 00:42.040 about the scattering from the sample than an unpolarized beam. And that

00:42.040 → 00:47.280 comes down to the way that the neutron interacts with the sample. There are two

00:47.280 → 00:51.360 different interactions here. So we have the electromagnetic interaction between

00:51.360 → 00:57.200 the neutron dipole moment and unpaired electron spins in the sample. So that's

00:57.200 → 01:02.560 magnetism. And we also have interactions between the neutrons and the

01:02.560 → 01:07.480 nuclei in the system. That happens via the strong nuclear force. And of course

01:07.480 → 01:13.160 nuclei can also have spins. But because of the fundamentally different origin of

01:13.160 → 01:19.000 these interactions, the different mechanisms, they have different

01:19.040 → 01:24.440 probabilities of changing the neutron spin state

in the scattering process. So

01:24.440 → 01:28.160 basically if we come in with a polarized beam and we look at the

01:28.160 → 01:32.600 polarization after scattering, we can work out how the neutrons have scattered.

01:32.600 → 01:37.800 And this is called polarization analysis and it's a large part of what we do

01:37.800 → 01:44.440 here at ISIS. Fantastic. So it seems like your speciality is polarized

01:44.440 → 01:51.040 neutrons. So as an instrument scientist here at ISIS, what does your day-to-day

01:51.040 → 01:55.320 work look like? Are you working mostly on the instruments? Are you in the

01:55.320 → 02:00.080 experiment hall? Are you working with users? Are you troubleshooting? Doing your

02:00.080 → 02:08.520 own research? I guess all of the above. Yeah, it's a very varied job. And you

02:08.520 → 02:13.760 often don't know what the day will bring. That's coming back to what you said

02:13.760 → 02:21.840 about troubleshooting. So I guess a typical day really depends on whether

02:21.840 → 02:26.160 the accelerator is running or not. So if the accelerator is running and we're

02:26.160 → 02:33.640 doing experiments, we spend a lot of time in the lab setting up equipment for

02:33.640 → 02:38.000 neutron scattering experiments on various instruments, running those

02:38.040 → 02:45.640 experiments and helping users analyze their data. When we're not running the

02:45.640 → 02:53.080 accelerator, the tasks are more in the direction of developing the

02:53.080 → 02:59.480 instrumentation. So say we want to put polarization analysis capabilities on

02:59.480 -> 03:03.800 another instrument, that requires some extra infrastructure that we need to

03:03.800 -> 03:08.760 design and implement on the instruments. And that is something that we do out of

03:08.760 -> 03:16.400 cycle. That time is also for my own research, which is in magnetism and in

03:16.400 -> 03:21.440 energy materials, both of which are very important application areas for

03:21.440 -> 03:26.000 polarized neutrons, as well as doing some teaching, sometimes in

03:26.000 -> 03:31.800 Stavanger or other places around the world. And I could go on and on and on.

03:31.800 -> 03:37.640 It's a very, very job. Recently we learned that you are going to be

03:37.640 -> 03:46.440 traveling to Japan and helping the Japanese team over the set up some

03:46.440 -> 03:53.040 instrumentation. Would you talk a little bit about that trip and in general the

03:53.040 -> 04:00.400 travel opportunities that such a role allows you? Sure. So first a little bit

04:00.400 -> 04:05.720 of background. We developed a polarization analysis option on an

04:05.720 -> 04:10.720 instrument here at ISIS a few years ago. This instrument's called LET and it's

04:10.720 -> 04:16.920 used to measure the dynamics of solids and liquids. So that's everything from

04:16.920 -> 04:26.440 water to battery materials where we're looking at how the ions move. Our team,

04:27.040 -> 04:32.680 sorry, our collaborators in Japan have recently built a similar option on a

04:32.680 -> 04:38.560 spectrometer there. And this is used to look at higher frequency, so faster

04:38.560 → 04:43.200 processes like lattice vibrations, which I believe is the topic of this podcast.

04:43.200 → 04:48.840 And there the idea is to separate those from magnetic scattering because those

04:48.840 → 04:54.080 two can often lie on top of each other in the experimental spectra. So I'm going

04:54.520 → 05:00.120 over to help them set up the instrumentation to do that and also to

05:00.120 → 05:05.760 write some code to help them analyze the data. And that'll take me to Japan for

05:05.760 → 05:13.640 two months. And coming back to the final part of the question, one of the real

05:13.640 → 05:18.520 pluses if you're into that kind of thing of a career in science is the

05:18.520 → 05:22.840 opportunities to travel. And that's especially the case in this kind of

05:22.840 → 05:30.520 central facilities work where as the users you often will go abroad four

05:30.520 → 05:34.680 or five times a year for experiments. And on the instrument scientists side,

05:34.680 → 05:41.440 you go away often for a few months to other facilities. So that could be

05:41.440 → 05:47.440 Japan or there's a lab called Oak Ridge in the US or to Grenoble in France

05:47.520 → 05:54.200 where there's a big lab and spend some time there and learn what other teams

05:54.200 → 05:56.080 are doing in your field.

05:57.080 → 06:03.560 Brilliant. I should also like to know what parts of your work you find most

06:03.560 → 06:08.080 interesting, what gets you out of bed in the morning and how that's changed over

06:08.080 → 06:13.400 the course of your career. If you look back to your bachelor's years and then

06:13.720 -> 06:19.440 your master's and postgraduate studies and so on, what's been your

06:19.440 -> 06:23.280 motivator for pursuing science in this field?

06:26.720 -> 06:30.560 It's not changed so much, I'd say, through the years. It's still the

06:30.560 -> 06:36.560 intellectual challenge of solving a difficult problem. Ultimately, though I

06:36.560 -> 06:42.000 like designing instrumentation, building it and so on, what really excites me is

06:42.000 -> 06:46.560 when we collect the first data set from that instrumentation. And in recent

06:46.560 -> 06:52.480 years, having worked more from the central facilities side of things than

06:52.480 -> 07:01.160 as a user. Actually, could I start again? Yeah. Right. So I think that's not

07:01.160 -> 07:05.800 changed so much through the years. What really still excites me is the

07:05.800 -> 07:16.320 intellectual challenge of solving a really hard problem. And I kind of lost

07:16.320 -> 07:17.360 the train of thought there a bit.

07:19.560 -> 07:20.760 We will break break.

07:26.720 -> 07:31.840 Yeah, so that hasn't changed so much through the years. It's still really the

07:31.840 -> 07:36.640 intellectual challenge of solving a really hard problem. That's what gets me

07:36.640 -> 07:43.000 up in the morning. And I guess what what I have kind of acquired is an

07:43.000 -> 07:48.320 appreciation in the last few years for instrumentation and the importance that

07:48.320 -> 07:55.440 has for for driving science forward. And what I really enjoy now as well is

07:55.440 -> 07:59.720 helping other scientists solve really hard problems. So providing the

07:59.720 -> 08:06.360 infrastructure for them to get to the bottom of difficult questions that

08:06.360 -> 08:12.400 may be previous techniques haven't been able to address sometimes even for

08:12.400 -> 08:17.040 decades. So so that's that's an additional sort of pleasure of doing the

08:17.040 -> 08:17.640 thing I do.

08:19.320 -> 08:25.640 So you mentioned that you're somewhat involved with some teaching. And of

08:25.640 -> 08:32.840 course you mentioned your trips abroad collaborating with other teams. What

08:32.840 -> 08:38.160 advice would you have for younger people out there who are thinking about a

08:38.160 -> 08:44.560 career in experimental physics? How would you how would you advise them? And

08:45.400 -> 08:47.640 what sorts of skills or

08:48.640 -> 09:01.200 hmm, yeah, I see what you mean. No, so I guess is what I would say is that that

09:01.200 -> 09:07.680 science is still a very human endeavor. It's something that's driven forward by

09:07.680 -> 09:14.640 collaboration by human relationships. And so if you're considering a career in

09:15.280 -> 09:20.880 science in general, I would encourage you to not worry so much about the area

09:20.880 -> 09:26.760 that you work in. Because I think there's something interesting at the frontier

09:26.760 -> 09:31.160 of every branch of science, but about the people that you're working with. Because

09:31.160 -> 09:38.520 that's really important. Aside from that experiment, I mean, not just in the

09:38.520 -> 09:43.440 literal sense, but try different things. So if you have a chance to spend a couple

09:43.440 -> 09:48.120 of months working with with one group on on say a project in condensed matter

09:48.120 -> 09:54.480 physics, and then another chance to spend some time in experimental particle

09:54.480 -> 10:01.800 physics, give it a go and see what suits you. So yeah, don't overthink the

10:01.800 -> 10:06.560 things in these things. Just try and try to have fun. Right, that would be my

10:06.560 -> 10:11.680 advice. And make sure you get good grades. Because there's no alternative.

10:11.680 -> 10:18.360 Good grades, good grades always help. Yeah, absolutely. But I think there

10:18.360 -> 10:23.920 really no substitute for enthusiasm. Yeah, so if you are interviewing for a

10:23.920 -> 10:30.160 position, certainly as an interviewer, that's one of the first things I look

10:30.200 -> 10:37.160 for. Because even if you don't have the right background and whatever willingness

10:37.160 -> 10:50.840 to learn and the motivation. Sorry. So even if you don't have, sorry, even if you

10:50.840 -> 10:56.400 don't have on paper the right background for something, motivation and willingness

10:56.400 -> 11:02.960 to learn really goes a long way. And it's something that I rate very highly when

11:02.960 -> 11:10.800 I interview students or other job back. I don't know. You know what I mean.

11:10.800 -> 11:19.680 Yes. Yeah. Fantastic. Break. Break. Well, thank you so much, Dr. Nielsen, for your

11:19.680 -> 11:25.320 time. It's been a valuable chat. And I'm sure our listeners appreciate it very

11:25.320 -> 11:27.640 much. Pleasure. Thank you.

### A.2.3 Dr. Jacob Wilkins

00:00.000 → 00:07.080 Okay, so now I'm sat here with Dr. Jacob Wilkins, who is a research software

00:07.080 → 00:16.220 engineer here at ISIS. He's doing a form of computational computing. So Dr.

00:16.220 → 00:19.600 Wilkins, would you tell us a bit more about what you're up to here at ISIS?

00:19.600 → 00:25.560 Yeah, so I'm a research software engineer, which basically means that I have the

00:25.560 → 00:30.800 knowledge of a researcher and a knowledge of a software engineer, and my job is

00:30.800 → 00:36.480 kind of to translate between the two. So I will get scientists coming to me and

00:36.480 → 00:41.000 saying, I have this problem. Can we get it done in software or I have this

00:41.000 → 00:46.000 software. Can you get it make it better? So when it comes to ISIS, I'm currently

00:46.000 → 00:52.600 working on developing the Horace neutron analysis code. So you get the all of the

00:52.640 → 00:56.920 numbers that come out of the neutron spectrometer, and you want to be able to

00:56.920 → 01:00.160 turn those into something which is paper-worthy. You need to get the plots,

01:00.160 → 01:04.960 you need to filter the data, you need to find the interesting features. And so my

01:04.960 → 01:10.960 job recently has been making that code go faster and also work in parallel so we

01:10.960 → 01:18.600 can exploit these massively parallel machines. So my specialty is in high

01:18.640 → 01:24.600 performance computing. So my job is to make codes go faster so that scientists can

01:24.600 → 01:29.960 get their work done in a more reasonable time.

And some of the data that we get

01:29.960 → 01:34.840 coming out of the machines is half a terabyte, which if you try and process

01:34.840 → 01:42.440 that normally might take a couple of hours. And we recently had a user use one

01:42.440 → 01:48.280 of my optimized codes and it went from taking six hours down to 48 minutes.

01:48.280 → 01:52.880 Which brings it down into reasonable times rather than waiting overnight. So we're

01:52.880 → 01:57.160 hopeful we can keep doing that and still get the right answer. But getting the

01:57.160 → 02:02.200 right answer is tricky. Right. So it seems like you're working in an area which is

02:02.200 → 02:09.280 perhaps often misunderstood or dare I say even overlooked. So what got you

02:09.320 → 02:18.600 interested in being a software engineer associated with a large experimental

02:18.600 → 02:25.880 apparatus such as ISIS? Well it's more the fact that so ever since I started

02:25.880 → 02:31.920 doing in my undergraduate for example I did computational physics and although

02:31.920 → 02:36.960 it was called theoretical physics the module itself was computational. And so

02:37.000 → 02:40.720 our laboratories were taught in Fortran and we would develop software as part of

02:40.720 → 02:44.040 that project rather than doing the experimental labs where they sit around

02:44.040 → 02:50.080 watching instruments. We would develop software and simulate real situations. And

02:50.080 → 02:55.920 it became clear to me over the course of that undergraduate degree and then that

02:55.920 → 03:00.840 actually the programming the software elements were really caught my interest

03:00.840 → 03:06.800 far more than the physics in some senses. And then I did my PhD which was

03:06.840 → 03:14.080 in physics and I was implementing new features into software and then running

03:14.080 → 03:19.880 those new features to verify that they matched experimental results. But for me

03:19.880 → 03:23.320 the running bit was not the interesting bit. The interesting bit was getting down

03:23.320 → 03:27.280 to the nitty gritty of solving the problems and trying to work out okay

03:27.280 → 03:32.200 so what is the best way to do this in the in the most logical way in a way that

03:32.200 → 03:36.480 we can actually use this make it friendly and useful to somebody who comes

03:36.480 → 03:44.200 along from outside the field and also how to get it fast because the problem

03:44.200 → 03:51.280 that we were doing was if you want to simulate a shockwave in a material which

03:51.280 → 03:58.680 was what my PhD was on you generally need a lot of atoms to be able to simulate a

03:58.680 → 04:04.760 shockwave moving through a material. Now in classical molecular dynamics that's

04:04.800 → 04:08.360 fairly easy you can just pump up the number of atoms to a million a billion

04:08.360 → 04:16.280 you don't care. In DFT you get  $n^2$  plus scaling so as soon as you go above

04:16.280 → 04:19.840 about 2,000 atoms you're already looking very high performance machines for a

04:19.840 → 04:24.960 very long time. Doing a million atoms we calculated to do the scale that we would

04:24.960 → 04:33.800 need using naive methods would be a couple I think it was three 23 times the

04:33.840 → 04:40.680 age of the universe in parallel on a standard computer so obviously novel

04:40.680 → 04:45.680 methods are needed and it turns out there was a method which didn't require

04:45.680 → 04:50.800 such a large structure and so we implemented that method and we managed

04:50.800 → 04:56.720 to solve some real problems mostly looking at shockwaves in silica for

04:56.720 → 05:02.400 geophysics purposes because obviously you get a lot meteorite impacts in silica

05:02.440 → 05:08.080 and if we want to be able to look at what if we want to look at high pressure

05:08.080 → 05:12.440 phases the way you have to do that in the lab because you can't sustain many

05:12.440 → 05:17.560 gigapascals of pressure I mean you can get 200 but if you want to go above 200

05:17.560 → 05:21.200 you really need to just hit it very hard and let the pressure take its way

05:21.200 → 05:24.840 through. So that's the way they do it in the lab and trying to reproduce that

05:24.840 → 05:30.440 obviously we wanted to have accurate simulations and the other problem is that

05:30.440 → 05:36.960 when you look at molecular dynamics the potentials are usually defined for nice

05:36.960 → 05:42.720 stable crystals at room temperature when you start hitting tens of thousands of

05:42.720 → 05:47.640 Kelvin and disordered states the nose potentials fall apart this is really why

05:47.640 → 05:53.960 we want the DFT because you need to be able to accurately measure what is

05:53.960 → 05:57.160 happening within that crystal and you can't just rely on classical potentials

05:57.400 -> 06:03.080 the potential we're using the BKS potential for silica actually when you

06:03.080 -> 06:07.840 hit it hard enough you enter fusion because the potential actually tails

06:07.840 -> 06:12.040 off to negative infinity on the left side as your distance approaches zero

06:12.040 -> 06:16.520 because you don't usually explore that regime it's designed for a nice stable

06:16.520 -> 06:20.600 crystal so you're actually running to real problems of computation where you

06:20.600 -> 06:26.280 just you can't you can make corrections but you start entering new

06:26.320 -> 06:31.960 domains of physics right and I think it's becoming obvious how important your

06:31.960 -> 06:38.280 work is but I should like to know do you also have flexibility to publish papers

06:38.280 -> 06:43.680 is that something that you're that's on your radar so publishing paper the idea

06:43.680 -> 06:47.160 of the original one the original ideas of research software engineers are wrong

06:47.160 -> 06:53.000 was the idea of somebody who doesn't need papers to progress in the field

06:53.120 -> 06:57.560 because obviously there's a researcher and now this is this is drawing on a

06:57.560 -> 07:02.480 particular role of research software engineering it's a very new title only

07:02.480 -> 07:08.280 really formed in the last 10 or so years and there are multiple branches some

07:08.280 -> 07:12.800 people see it as an everyday programmer who you can call in to just solve your

07:12.800 -> 07:18.640 research problem other people see it as I am a physicist who writes good

07:18.680 → 07:24.440 software so I want to implement research ideas into software so those are the

07:24.440 → 07:30.800 two extremes of the sort of role of research software engineer is either

07:30.800 → 07:35.200 somebody who is called in to assist research as a software engineer or a

07:35.200 → 07:43.280 researcher who does software engineering so it becomes a bit of a sort of a bit

07:43.280 → 07:49.440 blurry but yeah the idea in some in some rationales is the fact that you don't

07:49.440 → 07:53.400 need to publish papers you are attributed as being a developer and a

07:53.400 → 07:57.640 maintainer of the software and that is your reputation it carries you now

07:57.640 → 08:02.600 unfortunately government funding bodies don't necessarily see it this way and

08:02.600 → 08:06.800 they expect research software engineers to meet the same publishing standards as

08:06.800 → 08:12.600 other researchers while they might not necessarily run the new codes or develop

08:12.600 → 08:17.120 it or you know if they're just being maintenance of the code then it's a

08:17.120 → 08:22.160 very different aspect so it's actually a bit of a fuzzy question it depends on

08:22.160 → 08:27.320 who you are and what you define your work to be right indeed what you want to

00:00.000 → 00:07.960 So Doctor, what's the most interesting aspect of your work today and how has that changed

00:07.960 → 00:13.480 over the course of your career from when you were an undergraduate to PhD to postdoc and

00:13.480 → 00:22.600 so on? What's kept you motivated and what's been the reason that you've got out of bed

00:22.600 → 00:24.600 to go into work?

00:24.600 -> 00:30.640 I mean the key debate here is whether I bother to get out of bed to go to work. I would probably

00:30.640 -> 00:39.160 say that for me it is the flexibility of the job. I have worked in various different

00:39.160 -> 00:46.440 fields over the years. For example, like I say my masters and PhD were in DFT molecular

00:46.440 -> 00:54.680 dynamics including path integral molecular dynamics and other such things. My first postdoc

00:54.680 -> 01:02.800 involved working with implementing novel algorithms into an empirical pair potential

01:02.800 -> 01:10.280 molecular dynamics code which is quite a different branch. I was looking at electrostatics in

01:10.280 -> 01:17.600 empirical pair potential codes and I did a project while also working at postdoc implementing

01:17.600 -> 01:27.280 a mechanism for getting quantum assembly language into the input scheme for a quantum computer

01:27.280 -> 01:32.160 simulator which is quite a different job to work in a molecular dynamics I've done before

01:32.160 -> 01:39.360 and now I'm working developing software for neutron physics which again is far removed

01:39.440 -> 01:46.240 from what I've done so this is the aspect of I enjoy learning different elements of physics

01:46.240 -> 01:50.680 and I get to interact with people from all over different branches of physics with their

01:50.680 -> 01:55.560 own passions and interests and I get to feel that passion and also try and learn a bit

01:55.560 -> 02:00.800 about the physics as it goes on and for me the real motivating factor as to why I like

02:00.800 -> 02:07.560 software engineering and software at large is there's a very much a primitive problem

02:07.600 -> 02:11.760 solving element the same thing you get when you finally cracked that Sudoku or something

02:11.760 -> 02:17.320 like that when you've managed to you've been slaving at a problem and there is a rush of

02:17.320 -> 02:21.720 adrenaline and orphans when you finally get to crack it and that is really exciting to me

02:21.720 -> 02:27.640 and the thing is again you're always having to think about different problems in new ways

02:27.640 -> 02:33.720 and part of the experience that I learned is there are so many facets to software that you

02:33.720 -> 02:38.960 need to deal with you've got to think about okay so if a new programmer comes along how

02:38.960 -> 02:43.880 quickly are they going to pick up what I've written okay if a user comes along how do I

02:43.880 -> 02:50.240 make my work make their life easier rather than just being another obstacle in the way of what

02:50.240 -> 02:56.080 they're doing and when it comes to user interfaces what is the best way of explaining to someone

02:56.080 -> 03:03.080 how do I how do I make the problem tractable and also make it obvious to someone that they

03:03.080 -> 03:07.160 can or can't solve the problem they want to solve with what we've done and these are all

03:07.160 -> 03:12.760 different aspects and then you get on to the final bit of okay how do I put this into software

03:12.760 -> 03:18.360 how do I take what's written in the software and get it up to either of any of those standards

03:18.360 -> 03:26.160 that I've got and also running quickly and there is a I just like the varied aspects that we get

03:26.160 -> 03:32.320 from software when you're trying to solve a problem in it I'm sure the same is true of any

03:32.560 -> 03:36.720 physical or scientific domain you can think of you will always find your problems and your

03:36.720 -> 03:43.560 niches and try and work them out but for me the the the the joy is in having so many different

03:43.560 -> 03:50.400 aspects of problems learning many different branches of not even physics but mathematics and

03:50.400 -> 03:56.320 also you know I talked to friends who are bio-physicists doing different things in in their

03:56.320 -> 04:01.040 fields with mech it down makes and other things like that and you get to see a whole host of

04:01.040 -> 04:07.760 problems in a way that you wouldn't if you isolate yourself in a box and then what would you say to

04:09.520 -> 04:15.280 budding software engineers or budding material scientists or computational scientists what

04:15.280 -> 04:23.520 should they be focusing on or what sort of spaces available in fields so in terms of what I would

04:23.520 -> 04:27.360 say that's a bit of a difficult question I'm not sure I have a single unified answer because

04:27.360 -> 04:32.320 material science software engineering and so on is so different but I would probably say

04:33.680 -> 04:38.640 find your own niche find the pieces that you enjoy and work out what they are and

04:39.280 -> 04:45.440 don't be afraid to experiment with something and find that you don't like it it's fine to not like

04:45.440 -> 04:51.840 something you don't have to slave away to make yourself like it in terms of software engineering

04:51.840 -> 04:56.800 I would say try and keep a wide scope if you have learned a particular programming language

04:57.520 -> 05:02.880 try and learn a new one and just learn the basics and see okay how does this make me think

05:02.880 -> 05:09.760 differently to when I'm thinking in what might be your native language and in terms of openings in

05:09.760 -> 05:15.520 the field there are particularly there is scope for leaving academia for industry or for government

05:15.600 -> 05:22.880 roles I mean this is a government role so there is scope for that there is a lot of scope for

05:23.840 -> 05:33.760 exploring different you know software branches there is a lot there are you know a lot of jobs

05:33.760 -> 05:39.520 which you can move into industry because obviously software is used heavily in industry so in terms

05:39.520 -> 05:43.520 of just generalized skillset and where it can take you I think can take you a long way no matter

05:43.520 -> 05:49.440 what you want to do and a lot of fields in particular are only just coming around to the

05:49.440 -> 05:55.520 idea that maybe we do need software maybe we do need to analyze these terabytes of data by

05:55.520 -> 06:02.160 something other than hand and I think it's only going to be a growing field as we move deeper

06:02.160 -> 06:09.360 and deeper into more and more complex instruments more and more complex data and we're going to need

06:09.600 -> 06:16.240 software that will outlast the project well thank you so much for your time Dr Wilkins

06:16.960 -> 06:22.320 without a doubt your insights will be of great use to lots and lots of people.

00:00.000 -> 00:12.000 I'm sorry. If you've decided, you know, I've done my PhD in a particular field and you even after work in that field for three years, you feel like that's the only knowledge you have.

00:12.000 -> 00:24.000 There's always an opportunity to respect, to work out what you want to do and try something new. You are not locked into what you did at your master's level, at your PhD level.

00:25.000 -> 00:31.000 And I think this is something that a lot of people mistake for is they think it's sort of a sunken cost fallacy.

00:31.000 -> 00:45.000 They think I've spent three years in FieldX. I can never leave FieldX. And I think that is a big mistake because exploring new areas just means, yes, you have to do a bit of catching up.

00:45.000 -> 00:53.000 You have to make sure you're not retreading the work that's already been done, but finding someone who is in that field and talking to them and asking them and getting out there and out.

00:53.000 -> 01:02.000 You know, you can reach out to academics or

other people and just send them an email saying, hi, I read your paper on X.

01:02.000 -> 01:09.000 I don't quite understand how this fits into the context of what I'm doing and you can't. The worst that happens is they send you a rejection letter.

01:09.000 -> 01:22.000 I guess the real worst thing that happens will be their rude, but the odds of that are so slim that, you know, it's worth just, if you are interested in something and you've read something and you feel you don't understand it,

01:22.000 -> 01:28.000 it's fine to contact someone and ask them. There might be people in your department or there might be people at your university.

01:28.000 -> 01:37.000 It doesn't matter if you are a physicist in, you know, in crystal structure. You can go and talk to a biologist on the other side of the campus.

01:37.000 -> 01:45.000 They might you speak a different language, you know, in terms of what they talk about, but you can ask them and you can work out what you fit into.

01:45.000 -> 01:53.000 And I think these days actually it's becoming more and more necessary to be interdisciplinary when it comes to developing and furthering science.

01:53.000 -> 02:03.000 We need physicists to go and talk to biologists and say, here is what we can do. What can you do for us? What can we learn from you?

02:03.000 -> 02:10.000 And how can you help me and I help you? And the only way to get these things going is by actually going out there and talk to them.

02:10.000 -> 02:15.000 And people like to sit in their little box and say, I'm a physicist. I do physics.

02:15.000 -> 02:27.000 And there is a language barrier. And I think that actually one of the things that a research software engineer does is translate from, I think the difference between a research software engineer and a software engineer,

02:27.000 -> 02:41.000 is a research software engineer has the skills and knowledge within the research field to translate what a researcher wants into what a software engineer needs without having to have a middleman in between.

02:41.000 -> 02:51.000 And I think that is the real benefit that we're starting to see from research software engineers, people with a specialism in a field who run software.

02:52.000 -> 03:02.000 Because if you walk up to a random person in the streets and say, OK, we need these lattice vectors redirecting to a SIF format, it's a very simple job.

03:02.000 -> 03:14.000 But unless you know the language, you don't know what it means. And I think that these sorts of things, it's the language we use.

03:14.000 -> 03:24.000 And I think that learning how to speak another language, if you get an opportunity to go and listen to, again, taking an example of a biologist, if you get an opportunity to go and listen to a biologist's talk

03:24.000 -> 03:33.000 and you don't understand a word of what they're saying, don't just walk out and say, God, that talk was terrible, you can ask people what they mean and what they're talking about.

03:33.000 -> 03:43.000 And most people are really excited when someone asks about their research because really the reason why they're often in that field is because they're passionate about their research and they want to share with people.

03:43.000 -> 03:53.000 So don't be afraid to ask, don't be afraid to look stupid by asking a question which is, quote, unquote, obvious. Don't be afraid to make mistakes.

03:53.000 -> 04:07.000 Make sure that you learn from what you are doing and make sure that you are helping, either you can help them, they can help you, or mutually you can grow together.

04:07.000 -> 04:09.000 I think that's another big thing as well.

04:09.000 -> 04:21.000 I think that's a really important point, one about interdisciplinarity, because it's becoming clearer and clearer that

the problems of today and the problems of tomorrow are interdisciplinary.

04:21.000 -> 04:34.000 And we need to be able to speak more than one language in order to form this unified front on the avant-garde of science.

04:35.000 -> 04:47.000 Traditionally, I think people within hard sciences have been quite siloed and quite proud of the fact that they are experts in one particular area.

04:47.000 -> 05:02.000 But it's becoming increasingly obvious that the more skills you have, the more languages you speak and the more people you're able to get your ideas across to, the better it's going to be for science in general.

05:02.000 -> 05:13.000 I also feel that actually being a layman in a field, coming into it and talking to an expert, and then they say a load of gibberish you don't understand.

05:13.000 -> 05:20.000 And you say, what does this mean? What does this mean? What does this mean? I'm sure it gets tiresome for that.

05:20.000 -> 05:28.000 One of the things is it can also help them understand how to talk to people outside their field, because this is one of the big things in sciences.

05:28.000 -> 05:42.000 People can't communicate to those who aren't also experts in their field, and that is a really damaging thing for either talking to, say you've made a major discovery in physics.

05:42.000 -> 05:52.000 A journalist comes to you and says, what does it all mean? And then they misrepresent it because you can't explain it to somebody who isn't an expert.

05:52.000 -> 06:03.000 Being able to communicate with non-experts in your field, and actually for a lot of universities and certain government roles,

06:03.000 -> 06:13.000 there is an opportunity to go and deliver lectures to undergrads, or deliver outreach programs to school children even.

06:13.000 -> 06:21.000 How do you explain to a six-year-old how to code? This is a very different challenge to talking to someone who already knows the basics.

06:21.000 -> 06:32.000 So I think actually another good thing to do is to get out there, try outreach, try explaining what you do to laymen.

06:32.000 -> 06:42.000 There is a webcomic called XKCD where the author, Randall Monroe, wrote a book called Thing Explainer.

06:42.000 -> 06:55.000 And the idea of Thing Explainer is it only uses the 2,000 most common words in English to explain things such as the satin-five rocket, or as he calls it, up-goer-five, because he wasn't allowed to use anything else.

06:55.000 -> 07:05.000 And there is a challenge available on the internet to summarize your thesis using the 2,000 most common words in English.

07:05.000 -> 07:20.000 And I think this is a good challenge for anyone to try because if you can't explain your research simply, clearly, and concisely without having to use invented specialist language,

07:20.000 -> 07:30.000 you are never going to sell it to anyone outside of your field. And it's an educational experience trying to do that because, you know, you get as far as,

07:30.000 -> 07:37.000 when I explain molecular dynamics to people, I say you put a load of dots in a box and you wiggle them around until they fall into the right places.

07:37.000 -> 07:43.000 And I think that that is a perfect summary of  
90

07:43.000 -> 07:48.000 And they go, well, imagine electrons are also in the box and you wiggle them until they fall into the right places.

07:48.000 -> 07:56.000 And that's pretty much what it is. They don't need to know. They don't need to care about local density approximations and generalized gradient approximations.

07:56.000 -> 08:04.000 Nobody cares. Nobody cares about what you do. What they want to know is what is the crux of what makes it interesting as the core feature?

08:04.000 -> 08:14.000 What am I going to take away from this? And being able to talk to someone about that actually is a really challenging but useful experience.

08:14.000 -> 08:23.000 So I think challenging yourself to do these things and use everyday language to explain what you do is quite a fun challenge.

#### **A.2.4 Dr. Kirill Nemkovsky**

00:00.000 -> 00:09.120 so I am testing the recorder I'm testing the recorder hey hello you hear me I do

00:09.120 -> 00:15.760 hear you I hear you very well okay we are recording number 14 so I'm sitting

00:15.760 -> 00:23.240 here in Dr. Kirill Namkovsky's office who is a polarized neutron scientist

00:23.240 -> 00:29.760 polarized neutron scientist and he's been at ISIS for a few years so Dr.

00:29.760 -> 00:36.720 Namkovsky why don't you tell us a little bit about yourself so as she will talk

00:36.720 -> 00:43.000 told I am polarized neutron scientist at ISIS in a neutron and muon

00:43.000 -> 00:50.200 instrumentation development group the main part of my job here is to provide

00:50.200 -> 00:56.000 support for polarized neutron experiments and also to contribute to the

00:56.000 -> 01:00.920 development of new instrumentation which involves involves polarized

01:00.920 -> 01:09.200 neutrons right so what does your day-to-day work look like well it's a bit

01:09.200 -> 01:14.080 different first of all it depends whether it's in the cycle or between

01:14.080 -> 01:22.400 cycles in the cycle when we have users with polarized neutrons so we stay

01:22.400 -> 01:34.520 these users to well to maintain the polarized instrumentation and also

01:34.520 -> 01:40.460 sometimes for some general help to start measurements I don't know to mount

01:40.460 -> 01:48.080 samples cryostats and so on between that of course we have a lot of commissioning

01:48.080 -> 01:52.640 work because before we do something we have to prepare everything we have to

01:52.640 -> 01:58.760 make sure it's working also as I told there is essential part of development

01:58.760 -> 02:03.560 for new instrumentation and besides that of course it's highly welcome it's also

02:03.560 -> 02:09.080 interesting for me I do my own science so my research as a scientist independent

02:09.080 -> 02:16.960 on user activity right so you are not only supporting the science going on at

02:16.960 -> 02:23.360 ISIS but also conducting some of your own independent research yes and also of

02:23.360 -> 02:29.840 course I can't do it not only here and sometimes it's even easier because when

02:29.840 -> 02:35.240 we play for being time for at ISIS we it's general competition for everybody so

02:35.240 -> 02:40.160 we have the same chances as others as external users and it depends on the luck

02:40.160 -> 02:44.120 and sometimes it's easier to get been time somewhere else like recently in

02:44.120 -> 02:49.600 December I've been to Japan for my own been time and Japanese people were coming

02:49.600 -> 02:53.960 here for the beam time so it's a bit right changing it's an international

02:53.960 -> 03:00.320 collaboration yeah that's brilliant so I would like to ask you what aspects of

03:00.320 -> 03:07.280 your job do you find most interesting and with that how's that evolved over time

03:07.280 -> 03:13.000 from the time that you were a PhD student and a postdoc and then you were an

03:13.000 -> 03:20.960 instrument scientist in Germany so what features of your work keep you excited

03:20.960 -> 03:27.720 and interested in in the field I think I start from the point when I was PhD

03:27.720 -> 03:33.320 student so that time of course I did not do any support of users I was using

03:33.320 -> 03:38.720 myself and actually I was coming here the user and the only exciting thing was

03:38.720 -> 03:44.240 doing my own sign so I did not do anything else of course doing experiment

03:44.240 -> 03:49.960 itself was exciting but usually it's a short part of the work like you do one

03:49.960 -> 03:54.440 week experiment and then you spend half a year or maybe more for data reduction

03:54.440 -> 04:01.520 analysis writing the paper then when I moved to Germany when I became

04:01.520 -> 04:07.760 instrument scientist myself I started to work this users and originally I was not

04:07.760 -> 04:14.200 interested in this like I understood it's a part of job but I did not find it

04:14.200 -> 04:20.480 interesting before I started to do it but then I realized I like it and now I

04:20.480 -> 04:26.800 tell yes it's exciting and when it was a long shut down and then after a long time

04:26.800 -> 04:31.680 I got users again actually I was very happy first experiment with users after

04:31.680 -> 04:38.760 long break yeah now well we have also a lot of instrumentation things which are

04:38.760 -> 04:45.960 not related to users maybe it's not very exciting when you just do it but of

04:45.960 -> 04:50.160 course when you come to the point when something is produced according to your

04:50.160 -> 04:56.040 design and it works and sometimes it works better than expected I can imagine

04:56.040 -> 05:01.800 that that must be a very rewarding feeling is there anything that you would

05:01.800 -> 05:09.600 say to young scientists to people who are considering a career in experimental

05:09.600 -> 05:16.480 physics in instrument science any advice you would have for them I'm not sure I

05:16.480 -> 05:22.680 don't know any good like can particularly advice but I would say from my

05:22.680 -> 05:28.880 own experience listen to yourself like try to understand what you like because

05:28.880 -> 05:35.560 often people follow some general ideas like everybody goes there let's do the

05:35.560 -> 05:46.280 same try to find your own field where you're really happy thank you technical university of Munich and

00:03.160 -> 00:09.880 There are plenty of people doing physics and mathematics and like hearing the small numbers for me. It's a bit weird

00:10.320 -> 00:17.280 Yeah, like for me. It's no normal to have a lot of people who do mathematics physics chemistry material science

00:18.600 -> 00:25.380 Yeah, I think it depends from from country to country because for example in stavanger most people are interested in

00:25.920 -> 00:27.920 the oil industry

00:28.440 -> 00:30.440 Yeah, and

00:30.600 -> 00:32.600 With Norway and producing

00:33.000 -> 00:36.800 tuition fees now for foreign students previously was completely free

00:36.800 -> 00:43.400 So I am doing my masters completely free from now on. It's going to be 15,000 euros a year

00:44.040 -> 00:48.280 15,000 euros a semester. Okay quite a lot. So that will

00:50.600 -> 00:54.800 Not encourage more foreign students. It's for foreigners. It's not for native

00:55.200 -> 00:59.400 Not for native, not for EU. Okay, it's as it normally is the case

01:00.680 -> 01:02.680 So people are very worried in Norway

01:04.160 -> 01:07.200 Because our two year master program might have to be shut down

01:09.200 -> 01:14.520 Yes, and the university gets funding based on the number of students

01:15.400 -> 01:20.120 so if they don't get funding then they don't get funding for their research and

01:21.840 -> 01:24.200 That's obviously not in anyone's interest

01:25.800 -> 01:28.920 But yes, I think there is a general trend of

01:29.600 -> 01:32.560 fewer people going into fundamental research and

01:33.160 -> 01:35.760 opting for industry and jobs and

01:36.680 -> 01:39.440 Germany it's much more connected. So Germany has

01:40.120 -> 01:46.120 Well, at least until recently now, it's a bit also getting worse. Germany has very

01:47.840 -> 01:49.840 large industrial

01:50.440 -> 01:55.640 Area and many people go to industry after PhD even

01:56.160 -> 02:00.920 So I knew quite a lot of people who did PhD by us and then went to industry

02:01.400 -> 02:04.840 It depends on the area, but in Germany, it's quite often

02:05.240 -> 02:08.760 Do you think the quality of this science that they are producing is

02:12.720 -> 02:14.720 Compromised

02:14.720 -> 02:19.640 No, no, I mean when they did PhD it was normal. Okay, normal quality PhD

02:19.640 -> 02:23.640 I don't tell like incredible or whatever, but I cannot tell anything, but

02:25.120 -> 02:27.120 No, it's just a question of

02:29.160 -> 02:33.400 In science overall, there are not that many positions

02:34.600 -> 02:40.360 And number of positions decreasing the higher you go like there are plenty of

02:41.160 -> 02:44.280 PhD positions a bit less postdocs and

02:45.720 -> 02:48.640 Like if you want to become professors, there are only few

02:49.280 -> 02:51.880 So when you are young, there are a lot of positions

02:51.880 -> 02:55.840 So it's easy to get and the same time you understand it would be more difficult later

02:56.360 -> 02:58.360 and that's quite natural that

02:59.000 -> 03:05.920 Some or many of these people go to industry where they have these positions and also they want these people and

03:07.000 -> 03:10.280 I'm not quite sure because I was never involved in this

03:10.520 -> 03:16.560 But what I've heard industrial people they even coming to universities like to have a look for students

03:16.560 -> 03:18.560 So there is this connection

03:18.600 -> 03:20.600 They do this

03:21.440 -> 03:24.040 It's called an English in German. It's job bertha

03:25.360 -> 03:32.240 Like job markets when there are some days people from industry are coming to make make some

03:33.240 -> 03:37.800 Presentations exhibitions. Yes and try to convince people to come to them. Yeah

03:38.800 -> 03:45.120 And universities do it a lot and I wonder if it's interesting if it's good for

03:46.360 -> 03:51.680 The whole science ecosystem. I think it's okay because it allows to keep high enough

03:52.200 -> 03:53.680 number of

03:53.680 -> 03:55.080 students

03:55.080 -> 04:01.720 I mean students are not afraid to go for PhD because they know that then they can find another job if they don't like science

04:01.720 -> 04:03.720 They have options. Yeah, they have options

## **A.2.5 Student at ISIS**

00:00.000 -> 00:09.200 Right, I'm sat here with Kirill and a student of his named Polly who's also working here

00:09.200 -> 00:15.480 in the Appleton Laboratory and she's part of something called the Sandwich Programme

00:15.480 -> 00:20.920 with local universities. So Polly, why don't you tell me a little bit about yourself and

00:20.920 -> 00:23.240 how you ended up here?

00:23.240 -> 00:28.120 So I'm a student at the University of Nottingham. I've done three years of studying. I'm taking

00:28.120 -> 00:32.800 a year out to do this sandwich placement and then next year I'm going back to do my final

00:32.800 -> 00:38.560 master's year and then I'll get my degree. So I got interested in this because I did

00:38.560 -> 00:42.920 a few internships throughout my university and they're all sort of like, you should really

00:42.920 -> 00:47.720 have a look at doing a sandwich year. It looks really good, employers really like it. I also

00:47.720 -> 00:53.840 did a research internship this summer of my second year and I really liked that. I went

00:53.840 -> 00:59.600 back to uni after that internship and while I liked uni I missed doing a big focused project

00:59.600 -> 01:04.600 rather than having to just go to lectures and learn by listening. So I really missed

01:04.600 -> 01:08.440 that and also being able to take things in the direction I wanted to go to rather than

01:08.440 → 01:14.000 following somebody else's syllabus. So I thought I'll apply for a sort of research placement

01:14.000 → 01:18.000 year and then for an entire year I'll just get to do exactly what I like doing which

01:18.040 → 01:24.320 is a research project that I get to take in whatever direction. So I had a look and this

01:24.320 → 01:29.520 one came up which was my number one choice. I applied for it and I got in. So yeah, that's

01:29.520 → 01:34.760 how I ended up here. Brilliant. And what did you expect to be doing here and what are you

01:34.760 → 01:41.440 actually doing? So on the advertisement for the job it was talking about the magic box

01:41.560 → 01:48.560 which is basically this, it's called a magneto-static cavity. It's mu metal box with coils on it

01:48.920 → 01:53.520 which creates a really homogenous magnetic field environment in the middle and you can

01:53.520 → 01:58.640 put helium three cells inside and it basically increases their lifetime because the helium

01:58.640 → 02:03.560 inside these cells is polarized. So if you have a really homogenous magnetic field they

02:03.560 → 02:09.000 stay polarized for longer which is useful for our experiment. Oh and it also has a flipping

02:09.040 → 02:16.040 coil inside so that you can flip the polarization from up to down which is also quite useful

02:16.160 → 02:20.000 for the experiments. And to be fair that is exactly what I've been doing for the past

02:20.000 → 02:26.200 six months. I've been designing that. It's a lot of work on the computer running simulations

02:26.200 → 02:32.000 and things. Something else that I didn't anticipate doing was I've been working on little side

02:32.000 → 02:35.960 projects for other teams which is quite nice because then you get to do a variety of things

02:36.080 -> 02:40.400 if you get a bit stuck in a rut with one project you can move to another and you get to meet

02:40.400 -> 02:45.160 different scientists and hear about what they're doing. Also when we have experiments on during

02:45.160 -> 02:49.560 a user cycle I get to go and have a look and see what they're doing, talk to them about

02:49.560 -> 02:55.280 their research and usually they come from far off places from around the world so that's

02:55.280 -> 03:00.240 quite fun to hear about their institutions and what they do. Brilliant yeah a little bit

03:00.320 -> 03:07.320 earlier on we actually saw the magic box that you've been working on. Oh really? The one

03:07.320 -> 03:11.320 we have. Ah yeah yeah because my one's not been built yet. The one that's still in computer

03:11.320 -> 03:17.440 it's not produced. Ah I see. So the production of it is that someone else who's going to take

03:17.440 -> 03:22.440 over or are you going to do the engineering as well? So I'm just doing the design. I've

03:22.440 -> 03:26.520 just been running my simulations. I've come up with dimensions of what I want. We've used

03:26.560 -> 03:30.960 a model from the ILL that's already been made and we've sort of adjusted that model to fit

03:30.960 -> 03:36.840 our specifications. I'm talking to a guy named Peter Galsworthy who's been creating a new

03:36.840 -> 03:42.720 model using my dimensions so on CAD and stuff and then he's going to turn that into drawings.

03:42.720 -> 03:47.080 We send that off to outside contractors to make the different parts then that gets sent

03:47.080 -> 03:53.080 to us and we build it from the parts. Kind of like IKEA furniture but very scientific.

03:53.440 -> 04:00.600 Some part will be done by our technician Mark. Okay. So in-house. Yes. Final assembly in-house.

04:00.600 -> 04:15.560 Okay. Break, break. So have you always been interested in experimental physics and after

04:15.560 -> 04:22.880 having been here for a couple of months has it reinforced your interest in remaining in the

04:22.880 -> 04:30.920 field or are you being pulled in many different directions now? When I was in school physics

04:30.920 -> 04:36.680 was my least favorite subject until about sixth form when I had a physics teacher that had a bit

04:36.680 -> 04:40.600 of a crush on so I tried to be good at physics to impress him and then I realized that I wasn't

04:40.600 -> 04:44.680 actually interested in him and the physics was actually quite cool and then when I did that

04:44.680 -> 04:48.280 research internship that I was telling you about that's when I became more interested in

04:48.320 -> 04:53.640 specifically the experimental side of it. I like doing a bit of everything, a bit of like

04:53.640 -> 04:58.720 computing work, a bit of theory and like working with my hands as well. So experimental lets

04:58.720 -> 05:03.520 you do all three rather than really focusing in on one of those aspects which is a lot more

05:03.520 -> 05:07.520 enjoyable I think and yeah working here is definitely reinforced that's something I want to

05:07.520 -> 05:13.040 do. I've been talking to a lot of different people especially PhD students because obviously that

05:13.040 -> 05:17.320 would be the next step after university and some of them are really positive, some of them are

05:17.320 -> 05:22.360 really negative and all of them are like you should do my specialization so I'm not entirely

05:22.360 -> 05:27.320 sure what specifically I'm going to do it in yet but I think I do want to stay experimental because

05:27.320 -> 05:31.920 I do like that practical side that you can only really get with experimental physics. So it seems

05:31.920 -> 05:37.480 like this sandwich program has been really useful in helping you decide exactly what you want to

05:37.480 -> 05:44.080 do giving you some exposure in the field, getting your hands dirty and reinforcing your love for

05:44.120 -> 05:49.640 physics. Yeah definitely just the amount of different people who do different things that you

05:49.640 -> 05:54.640 can talk to here about what their career path has been and the advice that they can give you is

05:54.640 -> 06:00.520 really really good like I found that very useful and yeah obviously having that experience means

06:00.520 -> 06:06.600 that I feel a bit more confident in myself and my skills and being able to show potential PhD

06:06.600 -> 06:10.440 supervisors that I've done this is going to be very helpful it probably means I'm going to have a

06:10.440 -> 06:15.960 wider choice of projects to choose from because this will hopefully differentiate myself a little

06:15.960 -> 06:25.280 bit from the crowd. Very good, break. Carol anything you'd like to add as far as students working in

06:25.280 -> 06:35.520 industry, the sandwich year, how is Petya doing? Well Petya is doing very well. Actually we saw

06:35.520 -> 06:41.040 here is very promising candidate from the very beginning on the selection procedure and what

06:41.040 -> 06:47.400 we see now completely matching our expectations and maybe even a bit higher I have to tell.

06:47.400 -> 06:57.560 Yeah in general we have sandwiched students almost every year from different universities,

06:57.920 -> 07:07.840 Nottingham is only one of them. There were several students from BAS from maybe one more from Nottingham

07:07.840 -> 07:15.200 I think but they're coming from many different local universities like London, Bristol, whatever.

07:15.200 -> 07:19.760 Okay, thank you.

## A.2.6 Dr. David Voneshen

Right, so now I'm sitting in Dr David Venetian's office, who's an instrument

00:05.560 -> 00:12.680 scientist here at the ISIS Neutron on New York source. So Dr Venetian, why don't you

00:12.680 -> 00:16.940 tell us a little bit about yourself and what you do here. Hi, yeah, so I'm an

00:16.940 -> 00:20.880 instrument scientist on the Merlin instrument, so we measure excitations

00:20.880 -> 00:26.440 in materials. I've been here seven and a half years now, but I've only spent the

00:26.440 -> 00:31.200 three of those on Merlin. I was on LED before, which is similar, but it looks at

00:31.200 -> 00:40.040 lower-energy sorts of things. Right, and what's your journey been at ISIS so far?

00:40.040 -> 00:48.080 Right, so I came to ISIS first of all as a user, so during my PhD I did various

00:48.080 -> 00:51.360 experiments here, mostly actually diffraction to begin with, so looking at

00:51.360 -> 00:56.480 the structure of materials, and then once we'd figured out the structure, then

00:56.480 -> 01:01.000 we started towards the end of it, looking more at how vibrations were

01:01.000 -> 01:06.720 traveling through these materials. So I did those experiments on Merlin, and then

01:06.720 -> 01:12.280 as I was finishing my PhD they were advertising for a couple of jobs on the

01:12.280 -> 01:18.000 excitations group instruments. I applied, was lucky enough to get one, and then

01:18.040 -> 01:25.960 yeah, came in, did about five years on LED, and moved to Merlin in February 2020,

01:25.960 -> 01:32.800 which was fantastic. So as a Merlin instrument scientist, what do you do on a  
01:32.800 -> 01:37.400 day-to-day basis, and do you have enough time to pursue your own independent  
01:37.400 -> 01:43.320 research or write papers and so on? Yeah, I mean so at least in theory the  
01:43.360 -> 01:48.120 job's broken up into thirds, so about a third of my time is taken up supporting  
01:48.120 -> 01:53.440 users, about a third of my time is spent developing the instrument, and then about  
01:53.440 -> 01:58.840 a third of my time is spent doing my own research, and actually I'm seconded one  
01:58.840 -> 02:03.280 day a week to Royal Holloway University of London to sort of pursue my own  
02:03.280 -> 02:07.280 research and work with some of their researchers on helping them use new  
02:07.280 -> 02:16.840 instruments. So my research is mostly on thermoelectric materials, which are in  
02:16.840 -> 02:21.440 theory the things you can use to turn waste heat back into useful power, or you  
02:21.440 -> 02:25.520 can run them in reverse, you put an electric current through them, and you can  
02:25.520 -> 02:29.440 use them for solid state refrigeration. So I'm looking at those and trying to  
02:29.440 -> 02:34.600 figure out how we can make them actually useful, because at the moment they're not  
02:34.640 -> 02:39.760 very widely used. Unless you have a solid state wine chiller, because you don't want your  
02:39.760 -> 02:43.600 wine being shaken up, because there's no moving parts. Right, that actually sounds  
02:43.600 -> 02:49.480 really interesting to me, since my master's thesis is about doing

02:49.480 → 02:53.320 computational modelling of thermoelectric materials, looking at the

02:53.320 → 03:00.800 harmonic approximations for phonons, so can you tell me a little bit about what

03:00.800 → 03:06.840 the latest research is in the area? Yeah, I mean, well, so there's a lot of

03:06.840 → 03:10.960 interest in, so the harmonic approximation is where things behave like a

03:10.960 → 03:16.320 nice pendulum, but the most interesting physics for me at least is what happens

03:16.320 → 03:22.000 when that approximation starts to break down, because when you've got something

03:22.000 → 03:27.320 behaving like a pendulum, it just keeps doing that forever basically. And what

03:27.360 → 03:31.440 we're interested in particularly is anharmonic terms, because those allow

03:31.440 → 03:36.000 phonons to interact and disrupt the flow of heat through materials. And to get a

03:36.000 → 03:39.600 good thermoelectric, you're looking for something that's got the electrical

03:39.600 → 03:45.520 conductivity of a metal and thermal conductivity of a brick, and that's

03:45.520 → 03:51.400 quite the difficult materials problem. So yeah, I mean, some of the stuff we're

03:51.400 → 03:55.480 working on has been particularly looking at a lot of the good materials are made

03:55.520 → 04:02.000 out of very rare, heavy elements. So bismuth telluride is the classic example,

04:02.000 → 04:07.480 and I've been doing some work with people at the University of Reading where

04:07.480 → 04:11.800 we're trying to look at sulfide-based materials. Sulfur's a lot cheaper than

04:11.800 → 04:15.640 tellurium, and so that would be one way of helping to commercialise them is make

04:15.640 → 04:23.680 them a bit cheaper. And so for the students in the audience, I'm sure

04:23.720 → 04:30.560 they'd be interested to know what parts of your research and your work do you

04:30.560 → 04:34.680 find most interesting, and how has that changed over the course of your career

04:34.680 → 04:39.240 from your undergraduate degree to your post-graduate degree and where you are now?

04:40.920 → 04:52.680 That's a good question. So I would say in many ways, actually, I'm still doing

04:52.680 → 05:00.440 the things that I loved as a student. I really enjoy getting stuck into a bit

05:00.440 → 05:06.560 of data analysis and working on slightly different materials. That's one of the

05:06.560 → 05:16.320 nice things actually about being here. But so how has it changed? I guess these

05:16.320 → 05:20.960 days I do more supervision of people doing some of the actual data analysis

05:20.960 → 05:27.960 than I did when I was doing my PhD. But I still managed to find time to do some of

05:27.960 → 05:39.600 it myself. Yes. Very good. And finally, I'd like to ask, what advice would you have

05:39.600 → 05:45.560 for some of the budding scientists and physicists and perhaps instrument engineers

05:45.720 → 05:50.800 and instrument scientists out there? What should they be thinking about throughout

05:50.800 → 05:57.680 their educational journeys and beyond? And in general, what would you have to say?

05:58.880 → 06:05.120 If you can do some internships, because that was how I mean, part of the reason

06:05.120 -> 06:11.280 that I haven't changed that much is that I still I really enjoy what I actually do on

06:11.280 -> 06:17.000 a day-to-day basis. And I found that out through doing a couple of placements during

06:17.000 -> 06:21.680 my undergraduate, where I discovered some things that I really did not enjoy doing.

06:24.960 -> 06:32.920 And was bad at, like objectively terrible at. And that's actually quite an important part

06:32.920 -> 06:36.360 of doing some of these things. Because until you've had a go, you might think it

06:36.400 -> 06:42.440 sounds cool. And then it turns out, actually, that yes, either you're bad at it, or you

06:42.440 -> 06:49.160 don't enjoy it, or a combination of two. Whereas I did. So the final placement I did

06:49.160 -> 06:54.320 was at the Institut de la Langevin in Grenoble in France, which is the European

06:54.320 -> 06:59.480 Neutron Source. And there I got to work on a project where I got to work with an

06:59.480 -> 07:06.920 instrument scientist, and do a little bit of data analysis and yet discovered that

07:06.920 -> 07:11.880 actually that was the sort of thing I really enjoyed. Before that, I'd been thinking I

07:11.880 -> 07:17.000 wanted to be a particle physicist, but it turns out that I love having a bit of ownership

07:17.000 -> 07:21.920 over a project, being able to see it through from start to finish on a sort of sensible

07:21.920 -> 07:22.640 time scale.

07:22.800 -> 07:30.520 Right. That actually begs the question of whether you could compare and contrast the

07:30.520 -> 07:34.400 experience of working here at the Butterford, Ableton, Langevin, Grenoble.

07:35.520 -> 07:45.040 The view's not as good here. You know, the mountains are lovely. I, yes, it's it's a

07:45.040 → 07:52.200 slightly, it's a similarly international place here, although it's funded predominantly

07:52.200 → 07:57.840 by the UK. We've got lots and lots of international colleagues and lots of international users

07:57.840 → 08:11.040 as well. We, yes, actually how different is the culture? There are some management styles

08:11.040 → 08:16.840 which are different, but the fundamental driver I think is the same. You know, we're all here

08:16.840 → 08:23.720 to do the best science we possibly can, and that means some late nights and long weekends

08:23.720 → 08:30.040 down on the instrument. And that's definitely just as true there as it is here. Yeah, we

08:30.040 → 08:37.920 don't have as good a coffee options, shortage of restaurants, shortage of mountains. But

08:38.920 → 08:44.920 otherwise, at least as a student, I found them similar.

08:45.920 → 08:53.920 Very good. Well, thank you so much for your time, Dr Venetian, and we thank you for pushing

08:53.920 → 08:58.920 the avant-garde of science forward. Have a safe flight. Thank you so much.

### **A.3 Episode 3: ESS, Dr. Rasmus Toft-Petersen, and Dr. Diana Castro**

00:00.000 → 00:09.000 We shall begin. Welcome everyone to episode three of Shaking Matters with me, Shibl Gill.

00:09.000 → 00:17.000 This edition comes to you from Garchig, where we are attending the European Conference in Neutron Scattering.

00:17.000 → 00:22.000 Today I'm joined by three big names in the industry.

00:22.000 → 00:31.000 First of all, we have Diana Castro, who is Associate Professor of Material Science at the University of Stavanger.

00:31.000 -> 00:42.000 We also have Joanna Lewis from the Europeans Relations Source, and she is the Scientific Outreach Coordinator.

00:42.000 -> 00:57.000 And finally, we have Rasmus Toft-Peterson, affiliated with DTU, but he's the Lead Scientist on the Bifrost Instruments being built at the Europeans Relations Source.

00:57.000 -> 01:01.000 So first of all, welcome to all of you. Thanks. Thank you.

01:01.000 -> 01:09.000 And we'd like to begin with you, Joanna. Would you give us an introduction of who you are and what you do?

01:09.000 -> 01:17.000 Sure. Hi. So I work at the Europeans Relations Source, and there I'm responsible partly for public engagement.

01:17.000 -> 01:27.000 So talking to members of the public and schools and high school teachers about what's happening at ESS, the plans and the future to inspire next generation

01:27.000 -> 01:41.000 and people who live in especially the member states, so Sweden and Denmark, but also expanding that out to the host nation states of Sweden and Denmark and expanding out to the member states.

01:41.000 -> 01:53.000 And also I do what's called Scientific Outreach. So talking as well to our scientific communities and making sure that the information they need, some sort of communications point of view is available

01:53.000 -> 02:02.000 and doing what we can to ensure stakeholder engagement, so making sure the right people can talk to each other and they have the tools they need to do that.

02:02.000 -> 02:07.000 Very good. And Rasmus, same question to you. Who you are and what you do?

02:07.000 -> 02:24.000 Right. I'm the lead scientist on Bifrost, so that's what I spend most of my time on. So I work with the engineers and the technicians to make sure that what we're building at ESS, Bifrost specifically, performs optimally and is scientifically world leading.

02:24.000 -> 02:36.000 So I'm the scientific component of that collaboration. And along with the lead engineer, we coordinate the contribu-

tions from the five member countries of which Norway is one of them.

02:36.000 → 02:39.000 And some part of my time also do some science.

02:39.000 → 03:02.000 Brilliant. Fantastic. So Joanna, we've heard about the ESS project on some previous episodes as well. Since you are currently based in Lund, I think on site at the ESS, would you tell us, give us an introduction to what the project is and what stage of construction it's in at the moment and

03:03.000 → 03:06.000 do I say when it might come online?

03:06.000 → 03:22.000 Sure. So, yeah, I work in Lund where the machine is being built. So the large majority of the buildings are now constructed. So we have a tunnel, we have a building where the instrument halls are and where all the instruments will be.

03:22.000 → 03:36.000 And we also have the office buildings and the lab buildings. And now we're in the stage of installing things in those buildings. So the accelerator tunnel, we have the beginning of the accelerator is installed and being commissioned right now.

03:36.000 → 03:49.000 We've switched it on and the first 20 meters or so have been conditioned and now commissioned as well. So we have some beam and some proton beam, which is what the accelerator is going to be accelerating.

03:49.000 → 04:02.000 Then at the same time, we're installing things into the experimental halls. So in the experimental halls, we have three halls with the different instruments, short and longer instruments. And they're at various stages.

04:03.000 → 04:22.000 They're at various stages. So we have a few where there's a hut where the scientists will sit. There might be the main instrument cabin and also some of the neutron beam guides also being installed at the moment.

04:22.000 → 04:33.000 So you can see if you're able to stand on the top of one of our instrument halls and look down, you can see the full length all the way down to where the target is in the middle.

04:33.000 → 04:47.000 So the target at ESS, you might not be aware,

is an interesting part of ESS as a spallation source, the way that the target design is really new and really not similar to any existing targets.

04:47.000 → 04:58.000 So it's a wheel suspended from a kind of like a pendulum in this huge vessel that is rotating and will rotate in time with the pulse of the protons.

04:58.000 → 05:11.000 And so when you visit the experimental halls, you have this cylindrical room in the middle and then these instruments that come out from that in left and right out of the center.

05:11.000 → 05:26.000 Brilliant. And Rasmus, I wanted to ask you, so Joanna's told us about the proton beam. At what point and how does that proton beam turn into a neutron beam?

05:26.000 → 05:38.000 It does so in a couple of processes. So the first is the spallation process where the high energy protons, they smack into a tungsten block basically or actually an assembly of tungsten blocks.

05:38.000 → 05:49.000 And in terms of the nucleus, you kind of excite the nucleus, you bring it up to a high energy level and then you can think of it as a kind of evaporation of very fast neutrons.

05:49.000 → 05:56.000 And these fast neutrons, they are not very useful because they have a too high energy. The energy is too high to probe materials.

05:56.000 → 06:06.000 They have a characteristic length scale and energy associated with atomic distances and bonds between them. So mega electron volt neutrons are useless.

06:06.000 → 06:13.000 So what we then have is that we have a cold moderator and a thermal moderator on top and the neutrons, they then smack into that.

06:13.000 → 06:21.000 And like when you play pool, if you take a pool ball and shoot it into a cushion, the pool ball comes back with roughly the same velocity.

06:21.000 → 06:28.000 But if it hits another pool ball, it loses a large part of its velocity. And that's what a moderator does because there's a lot of hydrogen in there.

06:28.000 → 06:35.000 Hydrogen is basically a proton, has the same

weight as neutrons. So basically the neutrons are slowed down.

06:35.000 → 06:52.000 And then you have this pulse of slow neutrons emitted from this moderator and then we install plugs into the shielding construction that pick up some of these neutrons, the useful ones, and we reflect them in super mirrors and then we guide them to the sample.

06:52.000 → 07:07.000 Fantastic. So with all this talk about neutrons, I wonder, and I'm sure our audience is also wondering, what can you actually do with these neutrons? What's all this fuss about? Any of you?

07:07.000 → 07:22.000 Well, the great thing about neutrons is that they are, of course, neutral, which means they're very highly penetrating. So you use them to look inside objects and you can see the atomic, you can see them at the atomic scale.

07:23.000 → 07:38.000 Although that's a really positive thing, it means that because they're neutral, they're much harder to steer. So this is why we have to have this kind of two-step process because you can't accelerate them with magnets in the way you would with the protons.

07:38.000 → 07:47.000 So you have to, as Rasmus mentioned, you have these reflectors to just try and guide them in this nice straight line down towards where your sample will be.

07:48.000 → 08:04.000 Right. We also know that neutrons, they have a spin. Do you also make use of the fact that they have half-introduced spin in terms of the observations that we're making?

08:04.000 → 08:15.000 Yes, you do. Yes. So we use the fact that neutrons have the spin. They can then interact with magnetically-ordered lattices, basically, or basically anything magnetic in principle.

08:15.000 → 08:32.000 So you can use that to actually investigate magnetic materials. So the most simple magnetic material is iron. The iron dipole moments, they sit in an ordered way, they're all parked in the same direction, but there's much more complex materials.

08:32.000 → 08:40.000 And investigating those, the only way you can basically investigate those complex orders, magnetic orders, is with neutron diffraction.

08:40.000 → 08:49.000 And because the neutron is heavy, a neutron with the right wavelengths to probe these ordered structures also has a very low energy.

08:49.000 → 08:55.000 So that means it has a possibility to actually investigate the dynamics with very good resolution.

08:55.000 → 09:05.000 And that's very contrary to X-rays, where the right X-rays, they have a very large energy. So it's a massive challenge to investigate low energy dynamics.

09:05.000 → 09:16.000 Right. So these neutrons, they are chargeless particles, but they have an agnostic moment, and that makes them very useful for probing a variety of different materials.

09:17.000 → 09:34.000 So what are some of the biggest challenges? We know that this facility has taken a very long time to build and cost lots of money. What are the challenges in terms of creating a neutron instrument?

09:35.000 → 09:43.000 So it's a crazy neutron instrument. It is mainly, in many cases, to try to maximize the number of neutrons that hit the sample.

09:43.000 → 09:50.000 So if you like bifrost, investigate dynamics, one out of 100 million neutrons will create a signal.

09:50.000 → 09:56.000 So for each neutron you measure, you need to shine 100 million onto the sample, roughly speaking, of course.

09:56.000 → 10:02.000 So that means you need to optimize the flux, but you also need the amount of useless neutrons to be as low as possible.

10:02.000 → 10:08.000 So fast neutrons around the detectors needs to be stopped and absorbed, so they need to be very attentive to that.

10:08.000 → 10:18.000 But then you also need to make sure that your instrument is flexible, that it can investigate many different types of experiments.

10:18.000 → 10:23.000 So what's important and exciting with a facility like DSS is that it's a user facility.

10:23.000 → 10:33.000 So people have ideas and they apply to come in and do a certain experiment that they thought of, a committee chooses

which one to do, and then you do them based on merit, basically.

10:33.000 → 10:42.000 So that also means you have to kind of anticipate what people will need. And I think that's one of the main challenges, to do that anticipation.

10:43.000 → 10:48.000 Because it's hard, 10 years in advance, to predict what people will find interesting.

10:48.000 → 10:53.000 But it means that we have spent a lot of this time in conversation with all of those people.

10:53.000 → 10:59.000 So the people who will be the users or the groups who might use it in the future, they have been involved in the design of these instruments.

10:59.000 → 11:03.000 What are their needs going to be? What's the sample environment they need to look like?

11:03.000 → 11:11.000 And that's why we've come to conferences like this one here this week, because we need to be in up-to-date conversations with those people to make sure

11:11.000 → 11:17.000 that the needs of the users are in line with the way that we're designing and building and constructing these instruments.

11:17.000 → 11:20.000 And that keeps moving and keeps being up-to-date.

11:20.000 → 11:31.000 Right. So a question, Joan, I'm sure you get posed quite often. This facility obviously costs billions of euros to build.

11:31.000 → 11:40.000 What are the benefits for building this particular facility over other neutron facilities that exist in Europe?

11:40.000 → 11:43.000 For example, the high alert source in France.

11:43.000 → 11:52.000 Yeah, so the concept for ESS was brought about by the scientists many years ago, and they wanted to be able to do more and more things.

11:52.000 → 11:57.000 And one of the main questions they wanted to be able to address was this idea of the flux.

11:57.000 → 12:05.000 How can we have more and more neutrons that are going to be at the right energy at the right time?

12:05.000 → 12:15.000 In addition, was this move towards spallation sources away from the sources that have a nuclear reactor in them?

12:15.000 → 12:23.000 So those typically do have a high flux. So if you're not having a nuclear reactor, how can you get your spallation source to end up with this very high flux?

12:23.000 → 12:33.000 The way that ESS is solving it is by having this very, very powerful accelerator so you can get more and more protons leading to more and more neutrons.

12:33.000 → 12:44.000 Then there's various other things to do with how the neutron beam itself can be tuned, and this was part of the other demands that the scientists were calling on many decades ago.

12:44.000 → 13:01.000 So there's this proposal that we needed a new upgraded spallation source for Europe, and over the last 10, 15 years this has been about working together to build something that meets the future needs of all of these scientists.

13:01.000 → 13:10.000 So far we've seen at this conference that scientists are very good at communicating their findings and their work to other scientists.

13:10.000 → 13:28.000 But I wonder how they were able to convince governments and policymakers to invest this huge amount of money into a scientific instrument which perhaps might not be very obvious to people who are not very scientifically literate.

13:28.000 → 13:35.000 So how do you go about convincing policymakers to invest these large sums of money?

13:35.000 → 13:41.000 I mean it's a really important conversation that had to happen early on. It's obviously public money that's being spent on this.

13:41.000 → 13:53.000 But a lot of the politicians around Europe acknowledge that science and innovation is often what drives the economy ultimately and can drive innovation in their own countries.

13:53.000 → 14:00.000 And so they want to be at the forefront of there wherever they can, and we all know that requires time and investment.

14:00.000 → 14:09.000 We're happy often to invest in kind of blue

sky research, and policymakers do get that that is how things move on.

14:09.000 → 14:15.000 You can't always say what the tool you build today will impact it will have in 40 years.

14:15.000 → 14:21.000 So there has to be this kind of acknowledgement and discussion about blue sky research and why it's important and it costs money.

14:21.000 → 14:30.000 Alongside that then though comes the very real examples and we all need stories and examples to bring things to life to be able to visualize what that's going to look like.

14:30.000 → 14:41.000 And so I think over the years the ESS has been creating and discussing particular parts, areas of life that matter to everyone.

14:41.000 → 14:51.000 So we care about climate change, we care about sustainability and what are going to be the energy sources of the future, for example.

14:51.000 → 14:58.000 So there are definite areas of research where neutrons can really help to study those things.

14:58.000 → 15:05.000 So let's take for example something like hydrogen as a fuel source in the future.

15:05.000 → 15:09.000 This has been something which potentially has been talked about.

15:09.000 → 15:12.000 Can we fuel cars with hydrogen in the future?

15:12.000 → 15:16.000 There's lots of issues about having hydrogen in a gas form.

15:16.000 → 15:20.000 It can be very dangerous and takes up a lot of space, so how can you use that?

15:20.000 → 15:25.000 One of the great things about neutrons is that they're really powerful for studying hydrogen.

15:25.000 → 15:31.000 So we've been studying hydrogen for 20 years about how you can use it perhaps adsorbed onto polymers.

15:31.000 → 15:35.000 So that the polymer is the thing you input in your car, for example.

15:35.000 -> 15:43.000 And all of that research is just incremental, but it means you're able to tell these stories with examples of fuel cells.

15:43.000 -> 15:46.000 We can actually make them better or the battery inside the car.

15:46.000 -> 15:51.000 We can study, say, the lithium and how it moves inside a battery and improving batteries.

15:51.000 -> 15:55.000 So battery research is one that's had a lot of government investment into it

15:55.000 -> 16:01.000 because we can see the benefits of having better and safer and smaller and lighter and cheaper batteries.

16:01.000 -> 16:04.000 And so it's something that governments have been willing to put money into

16:04.000 -> 16:10.000 and nuclear sources is a great part of the story of continuing that research.

16:10.000 -> 16:17.000 In fact, we also have the example of the Apollo program, which at the time the general public is quite skeptical

16:17.000 -> 16:23.000 of spending those huge sums of money, but it gave us technological breakthroughs

16:23.000 -> 16:29.000 that we are benefiting from every single day, but they weren't first seen at the time,

16:29.000 -> 16:36.000 including, I think, computer networks originated from the Apollo project.

16:36.000 -> 16:42.000 But for this particular project, we know that it's a Greenfield project, which means that

16:42.000 -> 16:47.000 everything was purpose built for this facility.

16:47.000 -> 16:51.000 In fact, the facility is built on a Greenfield.

16:51.000 -> 16:56.000 So how did that freedom allow for the use of breakthrough technologies,

16:56.000 -> 17:04.000 allowing you to design the whole facility from the ground up?

17:04.000 -> 17:06.000 What were the benefits?

17:06.000 -> 17:09.000 I think that it certainly brings a lot of challenges.

17:09.000 -> 17:11.000 If you have nothing there to start with, you have to build everything.

17:11.000 -> 17:18.000 So you have to create the infrastructure to be able to get construction vehicles onto the site at the beginning.

17:18.000 -> 17:23.000 One of the first things we had to do was dig the tunnel for the accelerator,

17:23.000 -> 17:28.000 and also we put in these piles for where the neutron guides are.

17:28.000 -> 17:31.000 They need to be very stable, so they're actually resting not on the ground

17:31.000 -> 17:35.000 and not on the floor of the facility, but on these piles that go all the way down to the bedrock.

17:35.000 -> 17:38.000 So these are the kind of first things that you have to start doing

17:38.000 -> 17:40.000 if you'll build something on a Greenfield site.

17:40.000 -> 17:44.000 And of course, before all of that was the geological sampling of where is the right spot

17:44.000 -> 17:50.000 and what is the geology there and how can you make something that's hopefully not too maybe magnetic

17:50.000 -> 17:53.000 and nice and stable.

17:53.000 -> 17:58.000 But in terms of the benefits, it means that you can kind of be very creative with that space.

17:58.000 -> 18:07.000 We had a perimeter around it, but we didn't have to worry about existing infrastructure, for example.

18:07.000 -> 18:14.000 We didn't have to work around many, I don't know, big existing buildings.

18:14.000 -> 18:20.000 Often these things are built in a university and it's just expanded and expanded, for example,

18:20.000 -> 18:27.000 but we were able to start with a relatively empty field and build from there.

18:27.000 -> 18:34.000 And of course, I'm sure you were able to plan for a much bigger time horizon

18:34.000 -> 18:39.000 looking into the future as the facility expands and so on.

18:39.000 -> 18:45.000 And we certainly had to work a lot with the Swedish government and also with the municipality around Lund

18:45.000 -> 18:48.000 because we were trying to create a dream, right?

18:48.000 -> 18:57.000 We were trying to convince them that this field would one day have thousands of researchers coming on a regular basis.

18:57.000 -> 19:01.000 They needed to travel there, they would need to stay and then when they were there,

19:01.000 -> 19:04.000 they would eat and sleep and spend money.

19:04.000 -> 19:10.000 And similarly, with the whole construction process, often there were Swedish contractors being used

19:10.000 -> 19:15.000 and so that also generates an economy for the area.

19:15.000 -> 19:19.000 So all of these things with a long-term project like building a facility,

19:19.000 -> 19:23.000 you have to be able to be able to tell those very long-term stories

19:23.000 -> 19:29.000 and create in people's minds a future where their field is at the centre of it

19:29.000 -> 19:36.000 and try and help them imagine how that will be and the benefits to them.

19:36.000 -> 19:42.000 So for a facility of this scale, of course, we know that it's an international effort.

19:42.000 -> 19:46.000 That involves lots of different member states.

19:46.000 -> 19:50.000 For example, of course, we are lucky to have Rasmus from Denmark here.

19:50.000 -> 19:53.000 He's working on the bifrost instrument.

19:53.000 -> 19:59.000 Can you speak a little bit about the international scientific collaboration

19:59.000 -> 20:05.000 that's getting into creating this facility?

20:05.000 -> 20:11.000 Yeah, yeah. It is complex. That's the best way to describe it.

20:11.000 -> 20:16.000 So you have some partners, many of them are from existing facilities.

20:16.000 -> 20:19.000 They have some very specific expertise in neutron scattering

20:19.000 -> 20:22.000 and in neutron scattering instrument construction as well.

20:22.000 -> 20:24.000 They have all these experts and they are needed there

20:24.000 -> 20:30.000 because it's exactly in this greenfield site so there's not the infrastructure to do all that just from the get-go.

20:30.000 -> 20:34.000 So you have to build all that up and then come from the existing facilities.

20:34.000 -> 20:40.000 So in bifrost case we have PSI, that's a neutron scattering facility in Switzerland.

20:40.000 -> 20:44.000 We have IV in Norway where they had the killer reactor

20:44.000 -> 20:48.000 and we have LLB in France where they also had a reactor.

20:48.000 -> 20:53.000 Some of those are closed down so that's also good for them to work on the ESS.

20:53.000 -> 20:57.000 And then we have University of Copenhagen and DTU in Denmark.

20:57.000 -> 21:03.000 So there's a lot of this expertise and then they have to come together to design a lot of these things

21:03.000 -> 21:06.000 and actually also procure them and deliver them.

21:06.000 -> 21:12.000 So that is a big challenge to do something like this.

21:12.000 -> 21:17.000 But it has to be coordinated and you really have to use the expertise of your partners.

21:17.000 -> 21:20.000 That's a simple thing.

21:20.000 -> 21:25.000 And for you Joanna, obviously you're a science outreach professional.

21:25.000 -> 21:33.000 I wonder what impacts projects like this have on inspiring the next generation of physicists

21:33.000 -> 21:41.000 or engineers or archaeologists or data scientists and all of the other specialists that come with it?

21:41.000 -> 21:44.000 Yeah, I mean I believe it can be very inspiring.

21:44.000 -> 21:52.000 I think that if you take teenagers who are at school today across Europe, this is being built for them.

21:52.000 -> 21:54.000 This is the next generation's spallation source.

21:54.000 -> 21:56.000 It's not for all the people who are at this conference today.

21:56.000 -> 21:59.000 They'll get a fair chance to use it for a few years.

21:59.000 -> 22:03.000 But actually the future users at this facility are still at school.

22:03.000 -> 22:06.000 So I'd like them to be as excited about it as I am.

22:06.000 -> 22:12.000 If they choose to carry on studying science or research once they leave school,

22:12.000 -> 22:18.000 then this has been built for them so that they can use it to further the cutting edge of knowledge.

22:18.000 -> 22:22.000 And I do believe that can be in itself pretty inspiring.

22:22.000 -> 22:28.000 And anything of a grand scale can feel, has a kind of intrinsic wow factor.

22:28.000 -> 22:30.000 So it is on a grand scale.

22:30.000 -> 22:31.000 It is big and large.

22:31.000 -> 22:35.000 It's not as big and large as CERN, but CERN can be quite hard to get your head around.

22:35.000 -> 22:40.000 It's big enough to, you know, my kids are always asking, is it bigger than Ikea?

22:40.000 -> 22:41.000 Is it bigger than Copenhagen Airport?

22:41.000 -> 22:43.000 They want to know these things.

22:43.000 -> 22:48.000 So that, you know, I think is in itself has a certain wow factor.

22:48.000 -> 22:52.000 But from the nitty-gritty point of view, I think there's more to it than that.

22:52.000 -> 22:54.000 You mentioned archaeologists there.

22:54.000 -> 23:00.000 When I describe what ESS is and what it's for, I often use the word as a microscope,

23:00.000 -> 23:05.000 because it's a giant tool to look at small things and the bigger your microscope or your tool,

23:05.000 -> 23:08.000 the ironically the smaller the object you can study.

23:08.000 -> 23:12.000 But with the idea of it as being a microscope, my next question, especially to younger kids,

23:12.000 -> 23:14.000 is often, well, what would you want to look at?

23:14.000 -> 23:17.000 If you had the biggest microscope in the world, what is it you'd want to look at?

23:17.000 -> 23:21.000 Because that's the kind of question we want to be asking these people to get them curious themselves.

23:21.000 -> 23:26.000 And if you look at it from that way around, it's not that we've got a question we're trying to solve it,

23:26.000 -> 23:30.000 and then someone is going to answer it in 10 years, and then there's nothing else to do.

23:30.000 -> 23:32.000 It's not like that at ESS.

23:33.000 -> 23:38.000 We will be expanding it and using it so long as there's more questions that need to be answered.

23:38.000 -> 23:45.000 So as an example of how 21st century research really happens,

23:45.000 -> 23:49.000 it's not one man in a room with a whiteboard.

23:49.000 -> 23:53.000 This is not how science moves anymore.

23:53.000 -> 24:00.000 It is a huge international collaboration, and for a piece of knowledge to be moved on

24:00.000 -> 24:04.000 it takes a collaboration of people often from many different countries,

24:04.000 -> 24:10.000 and the thing that inspires them and that gets them going is asking the interesting questions.

24:10.000 -> 24:13.000 And that is what I think is inspiring to younger people.

24:13.000 -> 24:18.000 Brilliant. And as you speak about these younger people,

24:18.000 -> 24:24.000 can you talk a little bit about the opportunities for students at the ESS,

24:24.000 -> 24:29.000 and perhaps specifically for Norwegian students and researchers,

24:29.000 -> 24:35.000 do you foresee any work in that field?

24:35.000 -> 24:40.000 Yes, so we've been talking about this, about kind of projects that we have even now.

24:40.000 -> 24:45.000 There are areas that we are looking for people to come with ideas,

24:45.000 -> 24:47.000 and you can probably talk about some of the...

24:47.000 -> 24:52.000 We have our data management and software centre, which is in Copenhagen, for example,

24:52.000 -> 24:58.000 and I know that they're interested in anyone who wants to learn more about software

24:58.000 -> 25:03.000 and about programming, looking at data and using computing to understand data.

25:03.000 -> 25:06.000 There's opportunities for students there even at the moment.

25:06.000 -> 25:09.000 In addition, we obviously have our instruments,

25:09.000 -> 25:12.000 and probably Rasmus has some more examples of that.

25:12.000 -> 25:16.000 And then obviously in the future there will be programs of PhD students.

25:16.000 -> 25:19.000 We hope to start building programs like that.

25:19.000 -> 25:24.000 Maybe we'll be looking at having PhD programs from particular countries,

25:24.000 -> 25:31.000 where they can co-sponsor or co-provide research PhD placements,

25:31.000 -> 25:33.000 and we'd love to be involved in those collaborations.

25:33.000 -> 25:36.000 Did you want to add any, Rasmus, from your kind of..

25:36.000 -> 25:38.000 What do you think, from an instrument point of view,

25:38.000 -> 25:40.000 are going to be the student opportunities?

25:40.000 -> 25:42.000 Well, there are many in principle.

25:42.000 -> 25:47.000 If students want to contribute in designing equipment for neutron scattering,

25:47.000 -> 25:50.000 there are many options to do simulations, for instance,

25:50.000 -> 25:52.000 or virtual instrumentation, basically.

25:52.000 -> 25:55.000 So that is a fairly easy thing to do as a bachelor project.

25:55.000 -> 25:59.000 That's always a possibility to ask your supervisor nearby

25:59.000 -> 26:02.000 if there's an opportunity to do some instrumentation.

26:02.000 -> 26:06.000 They can reach out to us as well, both their supervisors and students.

26:06.000 -> 26:11.000 Another thing is also to try and do some neutron scattering at existing facilities.

26:11.000 -> 26:14.000 Because one of the real great things about neutron scattering,

26:14.000 -> 26:17.000 as Joe mentioned, is that it's a very collaborative environment.

26:17.000 -> 26:19.000 People are not in silos.

26:19.000 -> 26:21.000 You have to work together with people,

26:21.000 -> 26:23.000 and many people find that quite inspiring.  
26:23.000 -> 26:27.000 And especially in Lund, where we have Max IV and ESS close to each other,  
26:27.000 -> 26:31.000 there's an obvious opportunity to actually get that feel as a scientist,  
26:31.000 -> 26:33.000 as a young scientist as well.  
26:33.000 -> 26:35.000 You have to try it first.  
26:35.000 -> 26:40.000 And of course, with Norway being one of the member states,  
26:40.000 -> 26:46.000 I'm sure there will be some privileges for Norwegian scientists to enjoy.  
26:46.000 -> 26:51.000 And the last thing, and we'll close out here,  
26:51.000 -> 26:54.000 and I would like all of you to chime in on this one,  
26:54.000 -> 26:59.000 what ESS activities are you personally most excited about?  
27:03.000 -> 27:06.000 I think, I mean, there's lots to choose from.  
27:06.000 -> 27:08.000 It's quite fun being at a conference,  
27:08.000 -> 27:10.000 because you remember when you've got five parallel sessions,  
27:10.000 -> 27:13.000 you realise how many different things are happening right at the moment.  
27:13.000 -> 27:19.000 I think, because it's being built in front of us all the time from Lund,  
27:19.000 -> 27:25.000 it is quite exciting just to see each bit being stored bit by bit.  
27:25.000 -> 27:29.000 I have a real soft spot for the target wheel.  
27:29.000 -> 27:31.000 I just think it's wacky and cool.  
27:31.000 -> 27:33.000 I used to work at ISIS in the UK,  
27:33.000 -> 27:36.000 where the target is like the size of a packet of biscuits,  
27:36.000 -> 27:38.000 and you just throw protons at it,

27:38.000 -> 27:40.000 and then eventually it breaks, and then you get a new one.

27:40.000 -> 27:43.000 I love this idea that someone went from a packet of biscuits

27:43.000 -> 27:46.000 to a giant two-and-a-half diameter wheel that rotates,

27:46.000 -> 27:49.000 just hanging from this seven-metre shaft.

27:49.000 -> 27:51.000 So I think the target wheel is really cool.

27:51.000 -> 27:56.000 And we've done some nice sort of real chemistry on it recently,

27:56.000 -> 27:59.000 of coating it with fluorescent coatings, for example,

27:59.000 -> 28:02.000 so that when the beam hits, we'll actually see it glow,

28:02.000 -> 28:05.000 and then we know everything's working, which I just thought was quite nice.

28:05.000 -> 28:07.000 That must be quite exciting.

28:07.000 -> 28:09.000 And I saw it through a little window recently.

28:09.000 -> 28:12.000 I saw it spinning and glowing, and that was pretty cool.

28:14.000 -> 28:16.000 To me, it's the instrumentation.

28:16.000 -> 28:18.000 So to me, it's when we build the instruments,

28:18.000 -> 28:20.000 and some of these instruments being built at the SS,

28:20.000 -> 28:24.000 they will really be very strong, like orders of magnitude

28:24.000 -> 28:26.000 better than what we have today.

28:26.000 -> 28:32.000 And seeing that potential realized will be amazing, I think.

28:32.000 -> 28:36.000 The way the users will use these instruments will be, I think, new,

28:36.000 -> 28:40.000 and I think we'll see something we've never had a chance to see now.

28:40.000 → 28:42.000 So that will be exciting for me.  
28:44.000 → 28:45.000 Diana?  
28:47.000 → 28:50.000 Well, so you said the instrumentation,  
28:50.000 → 28:53.000 then of course I had to add on the materials.  
28:54.000 → 28:59.000 The higher flux will open opportunities to  
look at very small samples  
28:59.000 → 29:01.000 that were impossible to be studied before.  
29:01.000 → 29:06.000 Usually, if you want to have information about  
the dynamics in matter,  
29:06.000 → 29:10.000 it's very useful to have single crystals, like a  
diamond,  
29:10.000 → 29:13.000 so that you have more information.  
29:13.000 → 29:17.000 And then it's very difficult to get single crys-  
tals of many materials,  
29:17.000 → 29:21.000 or if you are able to get them, they're usually  
very small.  
29:21.000 → 29:25.000 So it means that if you can measure smaller  
samples,  
29:25.000 → 29:31.000 then you might find a lot of new physics in  
matter.  
29:32.000 → 29:37.000 Well, it certainly seems to be quite a lot of  
excitement about the ESS.  
29:37.000 → 29:41.000 I can definitely confirm that from the confer-  
ence.  
29:41.000 → 29:45.000 And with that, I'd like to thank our guests  
today,  
29:45.000 → 29:48.000 Brasmus, Diana, and Diana.  
29:49.000 → 29:52.000 We hope you have a lovely rest of your con-  
ference,  
29:52.000 → 29:54.000 and we'll catch you next time.  
29:54.000 → 29:56.000 Thank you very much.





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