Computational Solid State Physics

- **Instructors:** L. Boeri, S. Moroni

SAPIENZA
UNIVERSITÀ DI ROMA

Outline

- **General Information**
- **Getting to know each other…**
- **What is Computational Solid State Physics?** *Content of the Course*
- **Practical Details**
- **Questions**

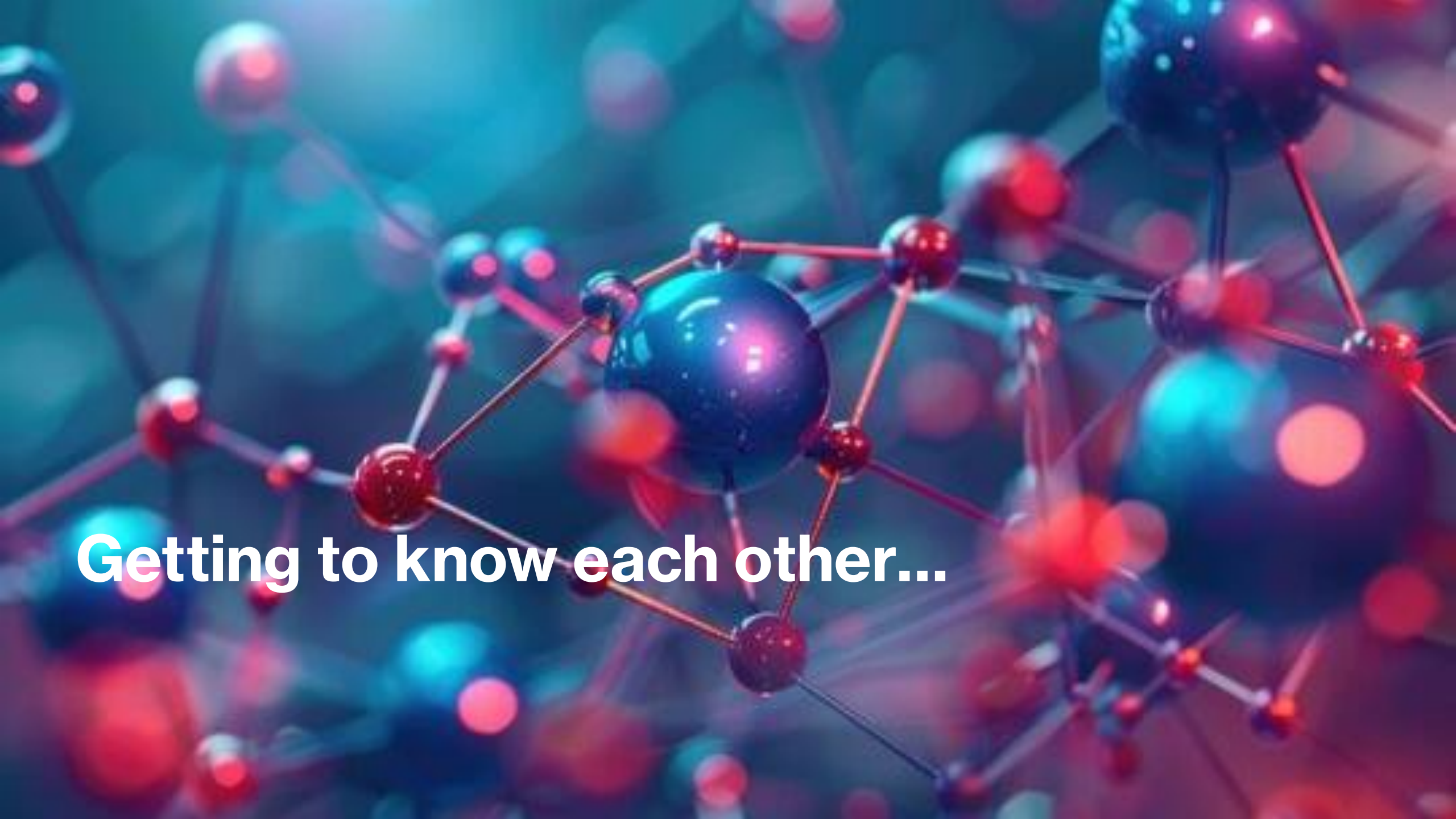
Practical Information:

- **Time and Place:**

Mondays: 10-14 Computer Room, via Tiburtina 205 (Lab. B. Pontecorvo)

Thursdays: 16-18, Rasetti lecture Hall, Marconi Building

- **Instructors:** Lilia Boeri, Saverio Moroni
- **E-learning:** https://elearning.uniroma1.it/course/view.php?id=16985
- **First Lecture:** Thursday, October 2nd, Rasetti Lecture Hall, 4 pm


Getting to know each other...

A few info about myself:

Lilia Boeri, Full Professor, Condensed Matter Theory, Physics Department, Sapienza, since April 2017.

Master (2001) and PhD (2005) in Physics, Sapienza.

Before coming back to Rome...

Graz University of Technology, Graz, Austria: Tenure-Track Assistant Professor (**2013-2017**).

Max-Planck Inst. for Solid State Research, Stuttgart (Germany): **Postdoc, Member of the scientific Staff and Max-Planck-Group Leader.**

Visiting scientist at: Duke University (USA); Riken (Japan); Naval Research Lab (USA); KITP-UCSB (USA).

Teaching:

National Scientific Habilitation (2017), Associate and full professor:
Thoretical Condensed Matter Physics, Theoretical Chemistry.

Lectures:

- Numerical Methods in Technical Physics (PHY.L20 & PHY.L30)
- Theoretical Solid State Physics I (515.468)
- Theoretical Solid State Physics II: Band structure methods

TU Graz

- Elementi di statistica per Fisica I per chimici (bachelor, 2016/17)
- Laboratorio di calcolo per fisici (bachelor, 2016/17 - oggi)
- Computing methods for physics (master, 2019/20 e 22/23)
- Condensed Matter II (master, 2020/21 -2022/23)

- Supervision of bachelor, master and PhD Theses in theoretical/computational condensed matter physics.
- Organizers of summer/winter schools on first-principles superconductivity (Goteborg, 2004; Duke, 2007; Vienna, 2017).

Research Activity:
Quantum Material Modelling Group, Sapienza

Computational Superconductivity: Use ab-initio (DFT) methods to understand and design new superconductig materials.

Why is it *useful*? Superconductors are promising materials for electrical grid components; they also have many other perspective applications in other fields (medical imaging, energy storage, quantum computing, etc)

Why is it *interesting*? Many fundamental questions on SC are still open, more than 100 years after their discovery. Numerical methods for SC, developed in the last 10-15 years, give a **microscopic understanding** on mechanism for SC in actual materials and allow design of better SC.

Recent Highlights:

Shedding light on old superconductors:

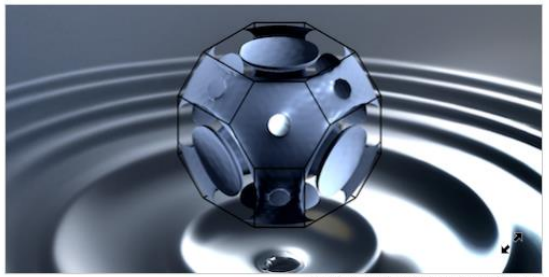
Physics ABOUT BROWSE PRESS COLLECTIONS Search articles

SYNOPSIS

Explaining Mercury's Superconductivity, 111 Years Later

November 3, 2022 • *Physics* 15, s155

Theorists have finally explained the superconductivity of mercury, the first superconductor ever discovered—gaining insights that could be relevant to the search for room-temperature superconductors.



Gianni Profeta and Cesare Tresca/University of L'Aquila

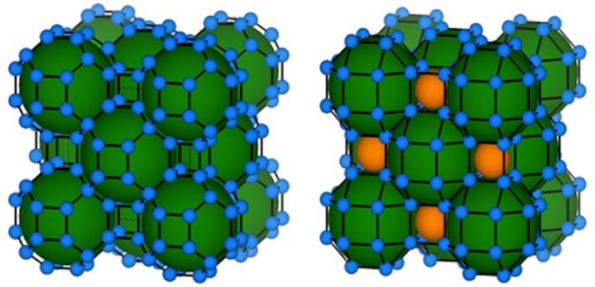
In 1911, physicist Heike Kamerlingh Onnes used liquid helium—whose production method he invented—to cool mercury to a few kelvins, discovering that its electrical resistance dropped to nil. Although mercury was later found to be a "conventional" superconductor, no microscopic theory so far managed to fully explain the metal's behavior and to predict its critical temperature T_C. Now, 111 years after Kamerlingh Onnes' discovery, theorists have done just that. Their first-principles calculations accurately predict mercury's T_C but also pinpoint theoretical caveats that could inform searches for room-temperature superconductors [1].

Designing new materials:

Physics — RESEARCH NEWS

Easing the Squeeze on Superconductors

Theorists propose new strategies for designing high-temperature superconductors that operate at vastly reduced pressures—a step toward ambient-condition superconductors.



(Left) Lanthanum decahydride (LaH_{10}) is one of the record-breaking, high-temperature, high-pressure hydrides that has been developed in recent years. The lanthanum atoms (green) exert a "chemical pressure" on the hydrogen atoms (blue), facilitating superconductivity. Researchers now show that the addition of boron atoms (orange) to the crystal, which results in the ternary compound $LaBH_8$ (right), can reduce the pressure needed to get high-temperature superconductivity.
Credit: L. Boeri/ Sapienza University of Rome

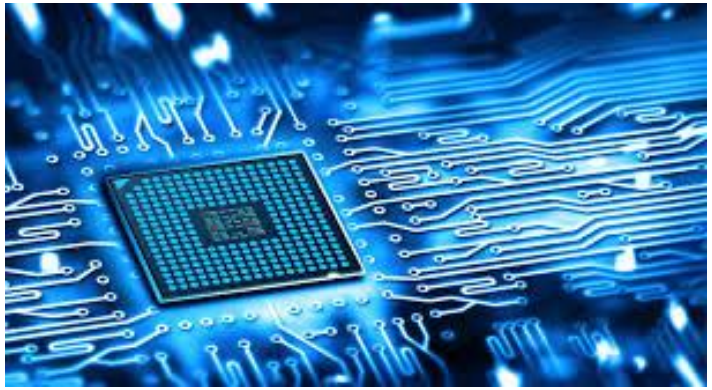
If you want to learn more: https://lboeri.wordpress.com

What is Computational Solid State Physics?

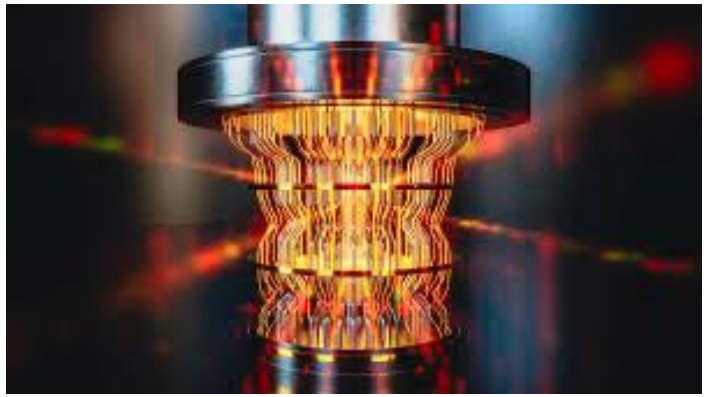
Aim of the Course:

The aim of the course is to give an introduction of the main numerical (**computational**) methods in **solid state physics**.

Computational Solid State Physics



Electronics



Quantum Computing

Superconductors

Photovoltaics

Spintronics

Computational Solid State Physics

The **fundamental problem** of solid state physics is to solve the **quantum many body problem** of interacting nuclei and electrons:

$$\hat{H}_{el} = -\sum_i \frac{\hbar^2 \nabla^2}{2m_i} - \sum_{\alpha,i} \frac{Z_\alpha e^2}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + E_{NN}(\mathbf{R}_\alpha, \mathbf{R}_\beta)$$

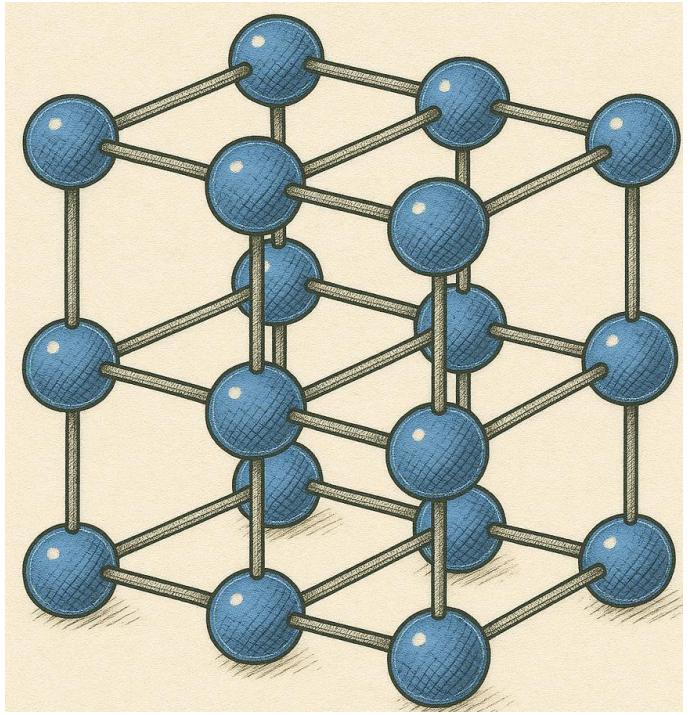
$\alpha = 1, ..., N_{at}$

$i = 1, ..., N_{el}$

$N \simeq 10^{23} - 10^{24}$

Computational Solid State Physics

Microscopically, a **solid** is a **regular arrangement** of atoms on a **periodic lattice.**



Bloch's theorem:

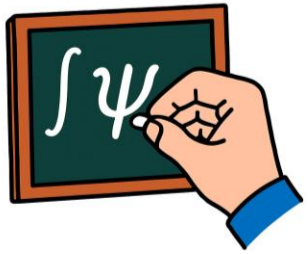
$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\, u_{n\mathbf{k}}(\mathbf{r})$$

$$u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$$

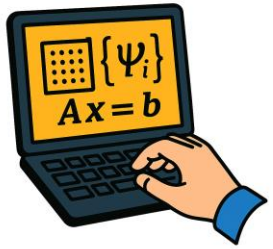
The Quantum-Many Body Problem:

$$\hat{H}\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = E\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)$$

Can be solved…



- **Analytically:** Only in very simple cases/limits



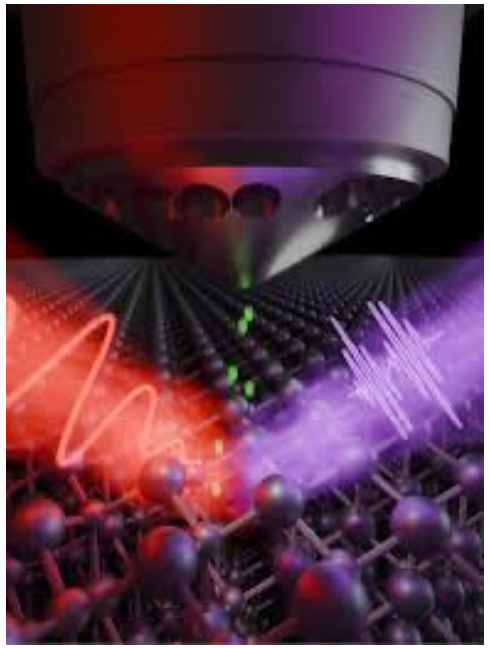
- **Numerically:** In all other cases, giving important material-specific insights

Computational Solid State Physics

Bridges the gap between experiment and analytical (many-body) Theory:

Experiments:

Complex Systems,
Direct Measurements

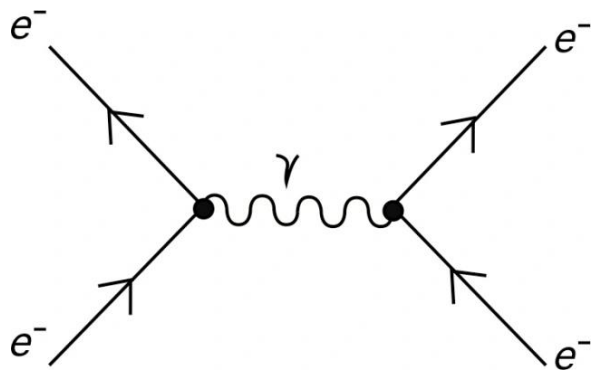


Computation:

Realistic Predictions,
Material Specific!

Theory:

Simple Models,
General Insight



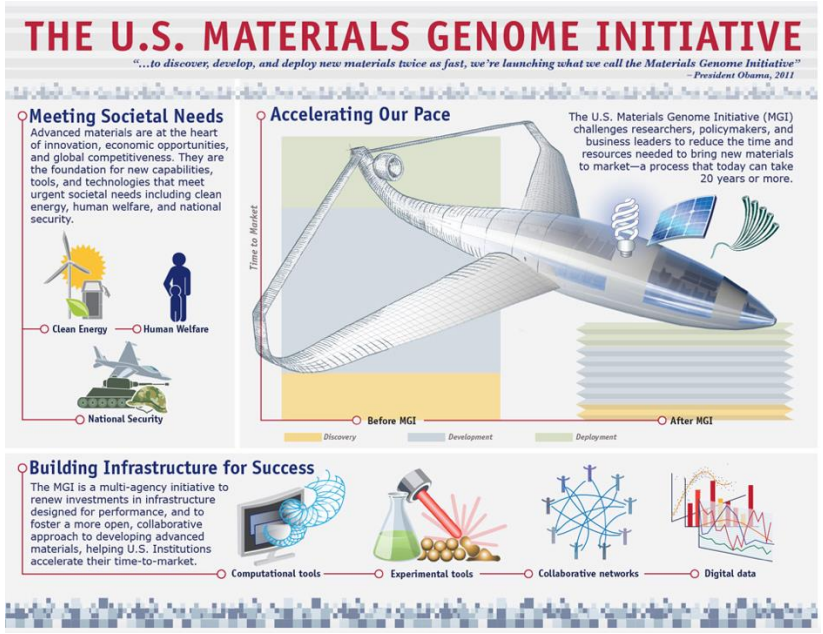
Computational Solid State Physics

Typical Questions:

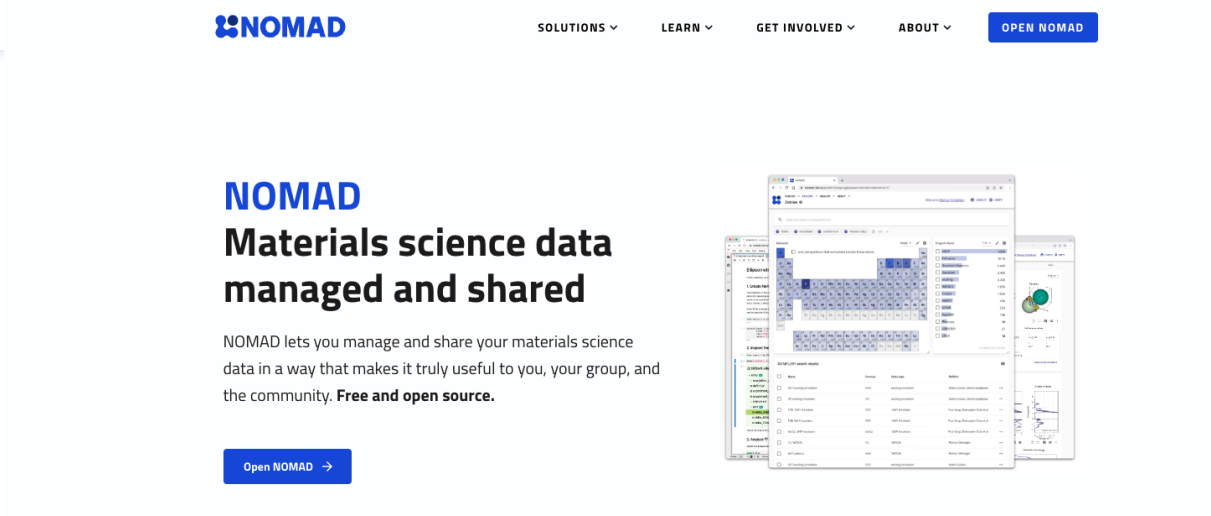
- Is this material a metal/insulator?
- What are the typical energies of a vibrational/electronic excitations?
- Can this material superconduct?
- Is it magnetic?
- Is it a topological insulator?
- Can these two/three elements mix and form a solid?
- What kind of solid will they form?
- What is the preferred structure?
- What is a supersolid?
- When will He become superfluid?
- What are the eigenstates of a given model Hamiltonian?

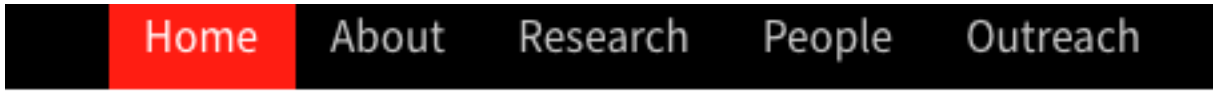
Computational Solid State Physics

Mapping the Material Genome...



https://www.mgi.gov/





MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Google Deepmind (Gnome DB)

SCIENCE

Millions of new materials discovered with deep learning

29 NOVEMBER 2023

Amil Merchant and Ekin Dogus Cubuk

Share

Lecture Content

Computational Solid State Physics

This lecture

Quantum Montecarlo (Part I)

Prof. Saverio Moroni

- **Dates:** 6th Oct. 2025 – 30th Oct. 2025 (Classes/Labs)
- **Midterm Test:** Nov. 3rd, 2025

Density Functional Theory (Part II)

Prof. Lilia Boeri

- **Dates:** Nov 6th, 2025 – December 15th, 2025
- **Midterm Test:** Dec. 22nd, 2025

Computational Solid State Physics

This lecture

Quantum Montecarlo (Part I)

- **Advantages:** High accuracy for complex quantum systems, including strongly correlated electrons, bosons, and quantum phenomena like superfluidity and quantum phase transitions.
- **Disadvantages:** Slow, limited system size, used only for simpler solids/models.

Density Functional Theory (Part II)

Advantages: Efficient for modeling electronic structure in large systems. Workhorse method in material science and industry for properties like band structures, vibrational properties, total energies.
Disadvantages: Accuracy can be limited for some type of systems (strongly correlated electrons). Cannot study quantum phase transitions.

Part I: Quantum Montecarlo (S. Moroni)

- **Stochastic integration, Metropolis algorithm**
- **Variational Monte Carlo:**

- Correlated wavefunctions, local energy
- Expectation values
- Optimization by correlated sampling

- **Projection Monte Carlo:**

- Imaginary time evolution

- **Diffusion Monte Carlo**

- Branching random walk, mixed and pure estimation
- Fermion sign problem and Fixed Node Approximation

Applications: Harmonic Oscillator, Electron Gas.

Part II: DFT in crystalline solids (Lilia Boeri)

- **Self-consistent field approximation.**
- **Density Functional Theory:** Hohenberg-Kohn theorems, Kohn-Sham equations.
- **Crystal structures and symmetry:** Space groups, Wyckoff positions, visualization using VESTA, use of the Bilbao Crystallographic Server.
- **Pseudopotentials** and their role in electronic structure calculations.
- **Electrons in crystals:** Brillouin zone, k-points, high-symmetry paths, and degeneracies.
- **Band structure and Density of States:** Computational methods and interpretation.
- **Total energy and interatomic forces:** The Hellmann-Feynman theorem.
- **Practical aspects of DFT calculations:** Basis functions, k-path setup, convergence testing, supercell calculations.
- **Advanced topics:** Crystal structure prediction, Machine Learning Interatomic Potentials.

Practical Details

Format of The Course

- **Front Lectures (Theory):** 20 Hours (Rasetti Lecture Hall)
- **Hands-on Sessions (Practical):** 40 Hours (Computer Lab, Via Tiburtina)

Hands-on-Sessions:

- **Quantum Monte Carlo:** In-house codes (C and Fortran)
- **Density Functional Theory:** Quantum Espresso Code (Plane-waves + Pseudopotentials)

All lecture Examples, Including Exam Tests, can easily be run on a standard laptop/pc

Exams:

- **Practical Computer Test + (Optional) Oral Exam**

The students will have the opportunity to take two tests in progress ("*prove di esonero*") at the end of each part of the course, or a final test after the end of the course. The mark **can** be improved taking an **oral exam**.

To pass the exam you are required to successfully pass both tests *in itinere*.

f you failed one or both tests, you have the possibility to take part in a practical test in January.

For students who will take the exam after the winter call, there is the opportunity to replace the written exam with a small (group) project.

Exams and tests are considered passed only if the mark is >=18/30.

Tentative Schedule:

- **Starting Date:** October, 2nd 2025
- **(Tentative) End Date:** December, 22nd 2025

First Test (QMC): November, 3rd 2025

Second Test (DFT): December, 22nd 2025

Makeup Test (DFT+QMC): January 12th 2026

- **Exam Session:** 19th Jan 2026-Feb 2026

Course Schedule (dates):

Oct	2 Intro	6 QMC LAB1	9 QMC TH1	13 QMC LAB2	16 QMC TH2	20 QMC LAB3	23 QMC TH3	27 QMC LAB4	30 QMC TH4
Nov	3 QMC TEST	6 DFT TH1	10 DFT LAB1	13 DFT TH2	17 SKIP	20 SKIP	24 DFT LAB2	27 DFT TH3	
Dec	1 DFT LAB3	4 DFT TH4	8 SKIP	11 DFT TH5	15 DFT LAB4	18 DFT TEST			

TO DO before the course:

- **Register on Elearning:**

https://elearning.uniroma1.it/course/view.php?id=16985

- **Equip your laptop with a Linux Distribution (**Virtual Machine or Dual Boot) or MaCOS

- **Install C, Fortran Compiler and Plotting Program** (Gnuplot, Python/Matplotlib, etc)

Questions?