



Teaching faculty Dr. Riccardo Mazzarello W2 Professor Institute for Theoretical Solid State Physics RWTH Aachen University, Aachen Germany



Course coordinator Dr. Anbarasu Manivannan Associate Professor Discipline of Electrical Engineering Indian Institute of Technology Indore Indore-453552 India

A TEN DAY COURSE ON

Fundamentals of Solid State Physics: From Theoretical and Computational Concepts to Recent Applications in Information Technology

F E B R U A R Y 5 - 16, 2018

Under the aegis of

MINISTRY OF HUMAN RESOURCE DEVELOPMENT

GOVERNMENT OF INDIA



Discipline of Electrical Engineering Indian Institute of Technology Indore Khandwa Road, Simrol Indore - 453 552



Course overview

Solid-state physics is an extremely important branch of physics from the point of view of applications. To name a few, the technologies of modern electronic devices - including its fundamental building block, the transistor - and of magnetic memories are based on the theoretical achievements of this discipline. The aim of solid-state physics is to determine the macroscopic properties of solid materials from the behavior of the microscopic constituents, namely molecules, atoms and electrons. Hence, the laws of quantum mechanics and statistical mechanics form the basis of this field. Important aspects of solid-state physics are the structural, mechanical and thermal behavior of crystalline solids, as well as their magnetic and optical properties. Nevertheless, it is the electrical properties that have drawn the most attention in the past decades and have led to spectacular advances in information technology.

The lecture course will provide an introduction to the most important such properties, including the structure and electronic structure of a crystal, its vibrational excitations, the electrical transport, and the magnetic properties, as well as to the theoretical concepts developed by physicists to elucidate these properties. Particular emphasis will be given to computational tools, in particular to *ab initio* methods based on density functional theory, which are the most widely employed methods to investigate solids. In the last part of the course, applications of some of these concepts to phase-change memories – a very promising technology for the realization of a "universal" non-volatile memory – will be discussed.

Course objectives

- Illustrate basic theoretical concepts of solid state physics and introduce selected first-principles computational methods to investigate solids.
- Introduce the audience to the manifold variety of properties of solids.
- Explain how phase-change materials and memories work and explore atomistic simulations.

Broad topics

- * **Introductory concepts:** Free-electron gas; Born-Oppenheimer approximation; Bravais lattices
- * **Bloch theory:** Bloch's theorem; electronic band structure of crystals: metals, band insulators and semiconductors; weak periodic potentials; tight-binding methods
- Coulomb interaction effects: Hartree-Fock theory; exchange and correlation energy; screening
- * **Electronic structure methods:** Density functional theory; plane waves and pseudopotentials
- * **Electrical transport:** Semiclassical theory; Boltzmann equation
- Vibrational properties: Introduction to phonons, ab initio calculations of vibrational properties
- Magnetism: Magnetic phases; model Hamiltonians; spin waves
- Phase-change materials: Structural, electronic and kinetic properties; applications

Some practical hands-on training sessions will supplement the lecture. These sessions will enable the students to make use of Quantum Espresso, a state-ofthe-art, open-source software based on the *ab initio* techniques introduced in the lecture.

Target audience and prerequisites

The course is meant for:

- * Students of undergraduate and graduate level (BTech/B.Sc, MTech/M.Sc., PhD students)
- BTech/B.Sc and MTech/M.Sc level teachers who wish to update their knowledge in an important field of physics

Any student/teacher with a basic background in quantum mechanics and statistical physics will be able to follow these lectures and gain valuable information. Familiarity with Linux would be a benefit for the practical sessions (but is not mandatory).

Faculty information

Prof. Riccardo Mazzarello received a PhD degree in condensed matter physics from the University of Hamburg (Germany) in 2004. He was a postdoctoral researcher at SISSA, Trieste (Italy) from 2004 to 2008 and at ETH Zurich (Switzerland) from 2008 to 2009. He was also visiting scientist at ICTP, Trieste (Italy) from 2004 to 2006. He became a junior professor in Theoretical Nanoelectronics at RWTH Aachen University (Germany) in 2009. There, he was promoted to W2 professor in Computational Solid State Theory in 2016. Since 2015, he is also adjunct professor at Xi'an Jiaotong University (China). His research interests include phase-change materials, surface physics, two-dimensional materials and opological phases of matter. He has contributed 59 peer-reviewed papers in the area of theoretical and computational solid state physics and condensed matter physics. According to Google Scholars, his works have been cited 10600+ times. He has given about 50 invited talks and seminars at conferences and research institutions.

Dr. Manivannan Anbarasu received a PhD degree from the Department of Instrumentation and Applied Physics, Indian Institute of Science, Bangalore (India) in 2008, for which he was awarded Dr. Srinivasa Rao Krishnamurthy Medal for the best Ph.D. thesis. From 2009 to 2012 he was an Alexander von Humboldt Post-Doctoral research fellow at RWTH Aachen University. From 2012 to 2016, he worked at IIT Indore as Assistant Professor of Electrical Engineering. In 2016, he was promoted to Associate Professor of Electrical Engineering at IIT Indore, where he is currently leading the 'Phase change memory research lab' for the development of ultrafast non-volatile memory, selectors and emerging electronic memory devices. Prof. Anbarasu is the coordinator for this GIAN course.

Course schedule

February 5, 2018	Introductory concepts
February 6, 2018	Bloch theory
February 7, 2018	Coulomb interaction effects
February 8, 2018	Electronic structure methods
February 9, 2018	Electronic structure methods
February 12, 2018	Semi-classical theory of transport
February 13, 2018	Phonons
February 14, 2018	Boltzmann equation
February 15, 2018	Magnetism
February 16, 2018	Phase-change materials

Registration fee

Participants from outside India	USD 500
Participants from the industry/corporate sector within India	INR 10,000
Participants from academia/research establishments within India	INR 5,000
Student participants from within India	INR 2,000

Application procedure

Step 1: Payment of registration fee

Payment of registration fee may be done online through NEFT transfer or offline through drawing a Demand Draft. Details for doing the same are as follows:

✤ NEFT transfer:

A/C No: 1476 1010 27440 Beneficiary name: Registrar, Indian Institute of Technology Indore Bank: Canara Bank Branch: IIT Indore, Simrol IFS Code: CNRB0006223 MICR Code: 452015003

Payment through Demand Draft:

Demand Draft should be drawn in favour of "Registrar, IIT Indore", payable at Indore.

Please send the Demand Draft at the following address. Do also send a scan of the Demand Draft at the email address provided below:

Dr. M. Anbarasu Associate Professor Discipline of Electrical Engineering Indian Institute of Technology Indore Simrol, Indore-453552, Madhya Pradesh Email: <u>anbarasu@iiti.ac.in</u> Mobile: +91-8085645649

Step 2: Registration

After completing the payment of registration fee, please fill out the application form available at: <u>http://gian.iiti.ac.in/register.php</u> Offline registration may also be done by filling out the adjoining form and sending it along with the Demand Draft. GIAN course on Fundamentals of Solid State Physics: From Theoretical and Computational Concepts to Recent Applications in Information Technology February 5 - 16, 2018

Registration Form

Personal Details:

Name of the Applicant :
Designation:
Affiliation:
Address for Correspondence:
Phone:
E-mail:
Details of Bank Draft:
Draft number:
Bank Name:
Branch Name:
Amount RsDated/
Accommodation Required:
YES: No:
Note: Accommodation can be arranged on payment basis

(Signature of Candidate)

Note: A photocopy of this form can also be used for the registration .