MATLS 4NN3/6NN3: COMPUTATIONAL MODELLING IN MATERIALS ENGINEERING

Instructor

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Course description

Get microscopic insight to the structure of functional materials used in photovoltaics, light generation, piezoelectronics and origin of their properties from atomic-scale simulations.

Course structure

12 weeks, 3 hrs/week: 1 hr lecture, 2 hrs hands on session (tutorials)

Module 1 (week 1–2): Fundamentals of density functional theory (DFT)
- elements of quantum mechanics
- *ab initio* approaches in historical perspective
- DFT shortcut
- self consistency problem
- basis set
- pseudopotentials
- software (Wien2k, VASP, ABINIT)
- Tutorial: VESTA building and visualization of simple crystal structures
- Tutorial: ABINIT under Windows/Linux, analysis tools

Module 2 (week 3–4): Prediction of basic material structure
- equilibrium structure
- phase stability
- phase diagram
- convergence and accuracy
- Tutorial: stable structure of Fe (bcc and fcc phases, magnetism)

Module 3 (week 5–6): Mechanical properties
- elastic properties
- equation of state (EOS)
- strength and fracture toughness
- Tutorial: lattice constant and bulk modulus of Si, convergence test, R code for EOS

fit

Module 4 (week 7–10): Optical and electrical properties
- band structure
- transport coefficients
- Tutorial: Band structure of GaAs and Si (direct vs indirect semiconductors)
- Tutorial: Charge transport and effective mass
- Tutorial: Band gap engineering in (InGa)N
- polarization
- piezoelectric properties
- Tutorial: Electromechanical coupling in ferroelectric ceramics $PbTiO_3$

Module 5 (week 11–12): Structural defects and impurities
- supercells
- structure relaxation
- formation energy
- defect electronic states
- Tutorial: Solubility of C in fcc-Fe and bcc-Fe
- special topic project (6NN3)

Graduate students (6NN3) are required to develop an individual or a small group project where they apply the learned techniques to solving a problem in materials science of their choice. At the end, students are asked to prepare a tutorial for undergraduate students.

Learning Outcomes

- Basic knowledge of quantum-mechanical concepts used in computational modelling of materials.
- Use existing DFT programs for the quantitative simulation of intrinsic material properties.
- Ability to develop structural models that capture relevant interactions for a material property in question.
- Know how to interpret computational results and compare between computational and experimental results.
- Efficiently utilize Linux-based multiprocessor servers for solving demanding computational and data-intensive problems.

Prerequisites and relevance to other courses

The material covered is largely self-contained, but an earlier exposure to quantum mechanics and solid state physics (MATLS 3Q03 Materials for Electronic Applications) is desirable. No extensive programming knowlege is required.

Evaluation

Activities	Contribution to the final grade	
	4NN3	6NN3
Participation (12 lectures)[a]	17%	14%
Participation (12 tutorials)[a]	33%	26%
Final exam	50%	40%
Special topic project	—	20%
Total	100%	100%

[a]MSAF is required for missing academic work

Recommended texts include but not limited to the following titles

- June Gunn Lee, *Computational materials science: an introduction* (CRC Press, Taylor & Francis Group, 2012). ISBN: 978-1-4398-3616-3 (Main text)
- David S. Sholl and Janice A. Steckel, *Density functional theory: a practical introduction* (John Wiley & Sons, 2009). ISBN: 978-0-470-37317-0 (Secondary)
- Efthimios Kaxiras, *Atomic and electronic structure of solids* (Cambridge University Press, 2003). ISBN-13: 978-0521523394 (Optional)

Notes: The text by Lee gives a great introduction to the quantum mechanics and DFT. The text by Sholl and Steckel complements with a good set of examples, but is more shallow in terms of the DFT theory. The book by Kaxiras is more general and cover many aspects of computational materials science apart from DFT.