Course title: "Computational nanoscience, modeling of nanomaterials using density-functional theory: a practical introduction"	Course code:

Type of course	Level of course	Year of study	Semester/trimester	Number of credits allocated (work-load based)	speciality
Lecture Lab classes	basic	any	2	1	any

Name of lecturer: Prof. Henry P. Pinto

Objective of the course (expected learning outcomes and competences to be acquired):

The impressive development of nanotechnology has already reached high controllability levels on the matter and it is clear that future technologies will depend upon our ability to manipulate atoms accurately in particular in the context of the bottom-up approach. These levels of "nanomanipulation" require powerful techniques with atomic resolution such as the scanning probe microscopy (SPM). Within the field of nanoscience, a deep understanding of the electronic properties of the studied nano-object probed with SPM techniques is often challenging. It is therefore essential to use theoretical simulations to help the understanding of experimental results. Indeed, density-functional theory (DFT) has opened the field of first-principles simulations to the emerging field of nanoscience. This state-of-the-art first-principles approach has already play a key role in the discovery and understanding of fundamental questions that arise in materials science. The following workshop has been prepared for anyone who is interested in computational simulations using density-functional theory (DFT) using the Vienna Ab-initio Simulation Package (VASP).

Prerequisites:

Medium level of Quantum Mechanics or Physical chemistry, basic level of programing and knowledge of linux or OSX is desired.

Teaching methods:

Interactive lectures alternating theory with hands-on sessions.

Lecture with multimedia presentation

Lab classes – calculations in the computer laboratory

Course contents

1. First overview of density-functional theory (*DFT*)
2. First calculations using DFT with VASP
   - 2.1 Isolated atoms.- study case: the Si atoms
   - 2.2 Charged atoms.- study case: the ion Cl^-
   - 2.3 Bulk systems.- study case: the rutile TiO_2
3. Nuts and Bolts of DFT calculations
4. Functionals and potentials.- study case: the rutile TiO_2
5. Phase transformations.- study case: rutile vs anatase TiO_2
6. Electronic structure calculations.- study case: rutile TiO_2 *vs* anatase TiO_2
7. Modeling surfaces.- study case: the rutile TiO_2 surfaces
6. Defects in surfaces.- study case: O vacancy on rutile TiO_2(110)
7. Introduction to STM and how to model with DFT.- study case the TiO_2(110)
8. Strong electron-correlation.- study case: TiO_2 and NiO
9. Beyond standard DFT and hybrid functionals

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Recommended reading:

A. Primary literature:

- D. Sholl and J. A. Steckel, *Density functional theory: A practical introduction* (Wiley-Interscience, 2009), 1st ed.
- R. M. Martin, *Electronic structure: basic theory and practical methods* (Cambridge University Press, 2004), 1st ed.
- J. M. Thijssen, *Computational Physics* (Cambridge University Press, 2007), 2nd ed.
- Georg Kresse, Martijn Marsman, and Jürgen Furthmüller, *The VASP guide* (Institut für Materialphysik, Vienna University, 2016). URL: http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html

B. Supplementary literature

- Stephan Kummel and Leeor Kronik, *Orbital-dependent density functionals: Theory and applications*, Rev. Mod. Phys. 80, 3 (2008).
- Martin Head-Gordon and Emilio Artacho, *Chemistry on the computer*, Phys. Today 61, 58 (2008).
- Kieron Burke et al., 2007, *The ABC of DFT* (Department of Chemistry, Rutgers University), URL: http://dft.uci.edu/doc/g1.pdf

Programs:

- ASE, URL:https://wiki.fysik.dtu.dk/ase/
- VESTA, URL: http://jp-minerals.org/vesta/en/
- Mathematica, URL: http://www.wolfram.com/mathematica/

VASP, URL: https://www.vasp.at

Assessment methods:

Participation in classes

Language of instruction: English