

Workshop III: Density-Functional Theory Calculations for Modeling Materials and Bio-Molecular Properties and Functions - A Hands-On Computer Course

Sunday October 30, 2005

6:00–12:00 *Arrival: informal get-together, registration and dinner*

Monday October 31, 2005

8:00–8:50 *Check-In/Light Breakfast (Hosted by IPAM)*

8:50–9:00 *Welcome and Opening Remarks*

9:00–10:00 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Basics of density-functional theory and fast guide to actual calculations

10:00–10:20 *Break*

10:20–11:20 **Karlheinz Schwarz** (Technische Universität Wien)
From APW to LAPW to (L)APW+lo

11:20–12:20 **Peter Blaha** (Technische Universität Wien)
Introduction to the WIEN2k code

12:20–1:00 *Lunch (on your own)*

2:00–6:00 **Peter Blaha** (Technische Universität Wien)
Installing the WIEN2k code and Practical session I: Testing the numerical accuracy I, and calculating bulk $E(V)$ curves

6:00–7:00 **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Poster parade: announcing the posters, 2 minutes per participant

7:00–12:00 *Poster Session with Dinner Buffet (posters will be on display until the end of the week)*

Tuesday November 1, 2005

8:30–9:00 *Continental Breakfast*

9:00–10:00 **Peter Kratzer** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Algorithms for total-energy minimization and forces

10:00–10:20 *Break*

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- 10:20–11:20 **Christian Ratsch** (UCLA)
Structure optimization, phase transitions, phonons
- 11:20–12:20 **Peter Blaha** (Technische Universität Wien)
k-point summation, electron temperature, and more
- 12:20–2:00 *Lunch (on your own)*
- 2:00–6:00 **Mahboubeh Hortamani** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Practical session II: Testing the numerical accuracy II, and calculating equilibrium structures, phase transitions frozen phonons
- 6:00–12:00 *Dinner break...and back to the computers*

Wednesday November 2, 2005

- 8:30–9:00 *Continental Breakfast*
- 9:00–10:00 **Martin Fuchs** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Comparison of different xc functionals
- 10:00–10:20 *Break*
- 10:20–11:20 **Jutta Rogal** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Charge densities, energy bands, density of states, and Fermi surfaces
- 11:20–12:20 **Karsten Reuter** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Bridging scales: Ab initio thermodynamics
- 12:20–2:00 *Lunch (on your own)*
- 2:00–6:00 **Mira Todorova** (University of Sydney)
Practical session III: Calculating charge densities, energy bands, and density of states
- 6:00–12:00 *Dinner break...and back to the computers*

Thursday November 3, 2005

- 8:30–9:00 *Continental Breakfast*
- 9:00–10:00 **Marcus Elstner** (Universität-GHS Paderborn)
QM/MM calculations and applications to Biophysics
- 10:00–10:20 *Break*

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- 10:20–11:20 **Karsten Reuter** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Bridging scales: Ab initio molecular dynamics and kinetic Monte Carlo
- 11:20–12:20 **Mira Todorova** (University of Sydney)
Calculating core-level shifts, surface core-level shifts, STM images
- 12:20–2:00 *Lunch (on your own)*
- 2:00–6:00 **Igor Ying-Zhang** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Practical session IV: Calculations for surfaces; surface structure, surface core-level shifts, and STM images
- 6:00–12:00 *Dinner break...and back to the computers*

Friday November 4, 2005

- 8:30–9:00 *Continental Breakfast*
- 9:00–10:00 **Peter Blaha** (Technische Universität Wien)
Spin-orbit coupling, magnetism, strongly correlated electrons: charge-, spin- and orbital ordering I
- 10:00–10:20 *Break*
- 10:20–11:20 **Karlheinz Schwarz** (Technische Universität Wien)
Spin-orbit coupling, magnetism, strongly correlated electrons: charge-, spin- and orbital ordering II
- 11:20–12:20 **Claudia Ambrosch-Draxl** (Karl-Franzens-Universität Graz)
Electron-phonon coupling
- 12:20–2:00 *Lunch (on your own)*
- 2:00–6:00 *Practical session V: Calculations on your own problems (with the help of all tutors)*
- 6:00–12:00 *Dinner break...and back to the computers*

Saturday November 5, 2005

- 8:30–9:00 *Continental Breakfast*
- 9:00–10:00 **Patrick Rinke** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Novel functionals and the GW approach
- 10:00–10:20 *Break*

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- 10:20–11:20 **Claudia Ambrosch-Draxl** (Karl-Franzens-Universität Graz)
Excited states: time-dependent DFT, self-energies in the GW approximation, and evaluating the Bethe-Salpeter equation
- 11:20–12:20 **Joerg Behler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft)
Comparison of different methods and codes:(L) APW, LMTO, PAW, pseudo potentials, gaussian, etc.
- 12:20–12:00 *Lunch (on your own) followed by rollerblading or biking at Venice and Santa Monica beaches*

