

Day I: Tuesday, June 23	
Time	Activity
8:00-8:45	Registration.
8:45-9:00	J. Sofo (Penn State): Welcome.
9:00-10:00	K. Schwarz (TU Wien): Density functional theory (DFT) and the concepts of the augmented-plane-wave plus local orbitals (APW+lo) method
10:00-10:30	Coffee break
10:30-12:00	P. Blaha (TU Wien): An overview of the new WIEN2k package.
12:00-13:00	Lunch
13:00-15:30	Exercise I: Getting started, struct file, init, scf, charge density, DOS, bands.
15:30-16:00	Coffee break
16:00-16:30	P. Blaha (TU Wien): Structure optimization, volume, atomic positions (forces), minimization.
16:30-17:30	Exercise II: Volume optimization, force minimization, supercells.

Day II: Wednesday, June 24	
Time	Activity
9:00-9:30	K. Schwarz (TU Wien): Magnetism (FM, FSM, AFM).
9:30-10:00	P. Blaha (TU Wien): Core-level spectra (XSPEC, ELNES).
10:00-10:30	Coffee break (Group picture will be taken outside of Hammond Bldg.)
10:30-12:00	Exercise III: Spectra (xspec and elnes).
12:00-13:00	Lunch
13:00-14:00	S. Cottenier (Ghent U.): Hyperfine Interactions
14:00-15:30	Exercise IV: Structure optimization, magnetism.
15:30-16:00	Coffee break
16:00-17:30	Lab I: Work on personal or suggested project.

Day III: Thursday, June 25	
Time	Activity
9:00-10:00	J. Sofo (Penn State): Optical Properties of solids with the WIEN2k package.
10:00-10:30	Coffee break

10:30-11:00	J. Sofo (Penn State): Transport coefficients.
11:00-12:00	Exercise V: Optic.
12:00-13:00	Lunch
13:00-13:30	S. Cottenier (Ghent U.): Relativistic Effects
13:30-14:00	F. Tran (TU Wien): LDA+U, Hybrid-DFT
14:00-15:30	Exercise VI: Magnetism, Spin-orbit, LDA+U.
15:30-16:00	Coffee break
16:00-17:30	Lab II: Work on personal or suggested project.
begin 19:00	Conference Dinner: Days Inn Penn State

Day IV: Friday, June 26	
Time	Activity
9:00-10:00	K. Schwarz (TU Wien): Large scale applications with WIEN2k
10:00-10:30	Coffee break
10:30-11:15	P. Blaha (TU Wien): Installation of WIEN2k, parallelization, Grid computing.
11:15-12:00	F. Tran (TU Wien): Advanced GGAs
12:00-13:00	Lunch
13:00-14:00	Lab III: Work on personal or suggested project.
14:00-15:00	Posters + Coffee: Discussion on the posters presented.
15:00-16:00	Round table: General discussion on WIEN2k. P. Blaha, S. Cottenier, K. Schwarz, J. Sofo, and F. Tran