

Day I: Wednesday June 24

Time	Activity
8:00-8:45	Registration.
8:45-9:00	Khuong P.Ong: Welcome. K. Schwarz (TU Wien): Density functional theory (DFT) and the concepts of the augmented-plane-wave plus local orbitals (APW+lo) method
9:00-10:00	Coffee break
10:00-10:30	P. Blaha (TU Wien): An overview of the WIEN2k package for beginners
10:30-11:45	Lunch
12:00-13:30	P. Blaha (TU Wien): Volume optimization, QTL, AIM
13:30-14:30	Coffee break
14:30-15:00	Exercise I: Getting started, struct file, init, scf, charge density, DOS, bands, FS.
15:00-16:30	Exercise II: Volume optimization.
16:30-18:00	

Day II: Thursday, June 25

Time	Activity
9:00-10:00	P. Blaha (TU Wien): Forces, structure optimization, supercells, surfaces, phonons, Berry phases, Wannier functions.
10:00-10:30	Coffee break
10:30-11:00	K. Schwarz (TU Wien): Magnetism (FM, FSM, AFM).
11:00-11:45	R. Laskowski (IHCP): Optical properties, BSE
12:00-13:30	Lunch
13:30-14:30	Exercise III: Structure optimization, supercells and surfaces, phonons
14:30-15:30	Coffee break- Poster section
15:30-16:30	P. Blaha: Installation of Wien2k, parallelization
16:30-18:00	Exercise IV: magnetism

Day III: Friday, June 26

Time	Activity
9:00-10:00	F. Tran (TU Wien): advanced DFT, Hybrid-DFT, LDA+U, GW
10:00-10:30	Coffee break
10:30-11:00	T. Yamamoto (Tokyo): Core level spectroscopy (AES, XAS, EELS, XMCD)
11:00-11:45	Exercise V: Core level spectroscopy (XSPEC, ELNES)
12:00-13:30	Lunch
13:30-14:30	R. Laskowski (IHCP): Relativistic effects, non-collinear magnetism (NCM)
14:30-15:00	Coffee break
15:00-16:30	Exercise VI: Spin-orbit coupling, LDA+U
16:30-18:00	Exercises VII: Optic, hybrid DFT, mBJ

Day IV: Saturday, June 27

Time	Activity
9:00-9:30	K. Schwarz (TU Wien): Hyperfine interactions
9:30-10:00	R. Laskowski (IHCP): NMR chemical shifts
10:00-10:30	Coffee break
10:30-11:45	Exercises VIII: Hyperfine interactions + NMR chemical shifts Round table: General discussion on WIEN2k: P. Blaha, T. Yamamoto, K. Ong, R. Laskowski, K. Schwarz and F. Tran
11:45-12:30	