

Elk workshop program

Monday 3-Sept-2018 (Density functional theory and LAPW)

09:00-09:20 Welcome: E.K.U. Gross
 09:20-10:20 ABC of DFT (K. Burke)
 10:20-11:20 The linearized augmented plane wave method (D. J. Singh)
 11:20-12:00 Coffee break
 12:00-13:00 EFG of DFT (K. Burke)
 13:00-15:00 Lunch
 15:00-16:00 Introduction to Elk (J. K. Dewhurst)
 16:00-16:30 Coffee break
 16:30-18:30 Exercises: Setting up the input and performing ground-state calculations (Dewhurst and Sharma)

Tuesday 4-Sept-2018 (Functionals and Magnetism)

09:00-10:00 Magnetism and spin: General overview (L. Nordstroem)
 10:00-11:00 Functionals: New and old (Leeor Kronik)
 11:00-11:30 Coffee break
 11:30-12:30 LDA+U method and non-collinear magnetism in LAPW (L. Nordstroem)
 12:30-14:30 Lunch
 14:30-15:30 Magnons (P. Elliott/Nisha Singh)
 15:30-16:00 Coffee break
 16:00-18:00 Exercises: Magnetism (N. Singh and Jose Flores)
 18:00-20:00 Trouble shooting + Dinner (J. K. Dewhurst and S. Sharma)
 20:00-21:00 Meeting of organizers

Wednesday 5-Sept-2018 (Time dependent density functional theory and linear response)

09:00-10:00 TDDFT: Introduction (E.K.U. Gross)
 10:00-11:00 MD+TDDFT (Ivano Tavernelli)
 11:00-11:30 Coffee break
 11:30-12:30 Real time propagation in solids (P. Elliott)
 12:30-14:30 Lunch
 14:30-15:30 Linear response and beyond with ELK (S. Sharma/Nisha Singh/Peter Elliott)
 15:30-16:00 Exchange parameter from Elk (A. Jacobsson)
 16:00-18:00 Trouble shooting (with snacks and coffee) J. K. Dewhurst+M. Fechner

Thursday 6-Sept-2018 (Many body perturbation theory and material search)

09:00-10:00 MBPT: Introduction (F. Bruneval)
 10:00-11:00 Cutting edge structure prediction (Jose Livas Flores)
 11:00-11:30 Coffee break
 11:30-12:30 Hedin equations and GW method (F. Bruneval)
 12:30-14:30 Lunch
 14:30-15:30 Wannier functions in Elk (A. Gerasimov)
 16:00-18:00 Material search tutorial (Jose)

Friday 7-Sept-2018 (Phonons, superconductivity and advanced)

09:00-10:00 Linear response phonons in LAPW (Dewhurst)
 10:00-10:45 Superconductivity overview: BCS, Eliashberg and SCDFD (A. Sanna)
 10:45-11:30 Coffee break
 11:30-12:30 Warm dense matter (A. Cangi)
 12:30-14:30 Lunch
 14:30-15:30 Practical aspects of phonons (M. Fechner)
 15:00-16:00 Coffee break
 16:00-18:00 Tutorial on wannier and phonons (M. Fechner + Gerasimov)