

7th International summer school on Computational Quantum Materials 2024 (1 May 2024)

Monday May 20, 2024

08:15	Shengrui Wang, A.-M. Tremblay	Welcome
08:30	A.-M. Tremblay	Short introduction to the School. Quantum Materials
09:00	M. Côté	Introduction to DFT and Density functionals
10:00	Break	
10:30	A.-M. Tremblay	Correlations in electronic structure and their signatures + second quantization #1
11:30	Xavier Gonze	Abinit code, part 1
12:00	Lunch	
14:00	Poster Session	
15:00	M. Côté, Xavier Gonze	Hands-on training: Abinit #1
16:00	M. Côté, Xavier Gonze	Hands-on training: Abinit #1
17:00	Break	
17:30	AM Tremblay	Many-Body refresher: Evolution operator, Time-ordered product, Green functions #2
18:15	AM Tremblay	Many-Body Refresher: Spectral weight, Self-Energy, Quasiparticles #3
19:00	Dinner	

Tuesday May 21, 2024

08:30	AMT	Many-Body Refresher: Coherent state functional integral #4
10:00	Break	
10:30	A.-M. Tremblay	Many-Body refresher: Source fields, Luttinger Ward, #5
12:00	Lunch	
14:00	Poster Session	
15:30	Xavier Gonze	Abinit code, part 2
16:15	M. Côté, Xavier Gonze	Hands-on training: Abinit #2
17:00	Break	
17:30	M. Côté, Xavier Gonze	Hands-on training: Abinit #2
19:00	Dinner	

Wednesday May 22, 2024

08:30	Agnes Valenti	Variational wave-functions and Neural networks
10:00	Break	
10:30	A.-M. Tremblay	Many-Body refresher: Lindhard function, TPSC and other approaches #6
12:00	Lunch	
15:30	M. Côté, Sophie Beck (Wannier 90), Véronique Brousseau, Olivier Gingras	Hands-on training: Abinit + Wannier90
17:00	Break	
17:30	M. Côté, Xavier Gonze	Hands-on training: Abinit + Wannier90
19:00	Dinner	

Thursday May 23, 2024

08:30	O. Parcollet	Dynamical Mean-Field Theory (DMFT)
10:00	Break	
10:30	O. Parcollet	Dynamical Mean-Field Theory (DMFT)
12:00	Lunch	
14:00	Nils Wentzell	Introduction to TRIQS
15:30	O. Parcollet, M. Ferrero, TRIQS Team	Hands-on training: TRIQS #1 Green functions, Lindhard, TPSC
17:00	Break	
17:30	O. Parcollet, M. Ferrero, TRIQS Team	Hands-on training: TRIQS #1 Green functions, Lindhard, TPSC
19:00	Dinner	

Friday May 24, 2024

08:30	Michel Ferrero	Introduction to Monte Carlo methods, Ergodicity, Detailed balance, biased sampling, variance estimate.
10:00	Break	
10:30	Michel Ferrero	Continuous-time Quantum Monte Carlo (CT-Int)
12:00	Lunch	
15:30	O. Parcollet, M. Ferrero, TRIQS Team	Hands-on training: TRIQS #2 DMFT for models, IPT, 2-orbital model.
17:00	Break	
17:30	O. Parcollet, M. Ferrero, TRIQS Team	Hands-on training: TRIQS #2 DMFT for models, IPT, 2-orbital model.
19:00	Dinner	

Weekend, no class

