

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	A.-M. Tremblay	Many-Body refresher: Evolution operator, Time-ordered product, Green functions #2
18:15	A.-M. Tremblay	Many-Body Refresher: Spectral weight, Self-Energy, Quasiparticles #3
19:00	Dinner	

Tuesday May 21, 2024

08:30	A.-M. Tremblay	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	Michel Ferrero	Introduction to Monte Carlo methods, Ergodicity, Detailed balance, biased sampling, variance estimate.
12:00	Lunch	
14:30	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	O. Parcollet	Dynamical Mean-Field Theory (DMFT)
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	

Monday May 27, 2024		
08:30	David Sénéchal	Cellular dynamical Mean-field theory, exact diagonalization and results of a recent application.
10:00	Break	
10:30	Sophie Beck and Alex Hampel	Ab initio description of strongly correlated materials: combining density functional theory plus dynamical mean-field theory
12:00	Lunch	
14:30	N. Wentzell, S. Beck, A. Hampel	Hands-on training: TRIQS #3 Realistic DMFT with Wannier in TRIQS DFT tools
17:00	Break	
17:30	N. Wentzell, S. Beck, A. Hampel	Hands-on training: TRIQS #3 Realistic DMFT with Wannier in TRIQS DFT tools
19:00	Dinner	
Tuesday May 28, 2024		
08:30	F. Kugler	DMFT solvers: NRG / DMRG
10:00	Break	
10:30	M. Ferrero	Diagrammatic Monte Carlo : Introduction and Hubbard [slot 1]
12:00	Lunch	
14:00	K. Haule	Diagrammatic Monte Carlo : Coulomb gas [slot 2]
15:30	Break	
16:00	M. Côté, O. Gingras	Hands-on training: Abinit + DFT+DMFT
17:30	M. Côté, O. Gingras	Hands-on training: Abinit + DFT+DMFT
19:00	Dinner	
Wednesday May 29, 2024		
08:30	P. Werner	Nonequilibrium dynamical mean-field theory
10:00	Break	
10:30	Martin Eckstein	Diagrammatic theory for correlated electrons out of equilibrium
12:00	Lunch	
14:00	Alessandro Toschi	Diagrammatic extension of DMFT: Spin Fluctuations, Pseudogaps and Superconductivity
15:30	Break	
16:00	Anna Kauch	Two-particle response with parquet equations
17:30	Coffee break & free time	
19:00	Dinner	
Thursday May 30, 2024		
08:30	Gabi Kotliar	Successes and challenges in the electronic structure of correlated materials towards theoretical spectroscopy and materials design
10:00	Break	
10:30	Sangkook Choi	LQSGW+DMFT and the fully self consistent GW+EDMFT
12:00	Lunch	
15:30	Gabi Kotliar and Nicola Lanata	Connecting wave functions, auxiliary particles and quantum embedding methods
17:00	Break	
17:30	Nicola Lanata	Gutzwiller RISB + ghosts and its applications to models, electronic structure and non equilibrium systems.
19:00	Dinner	
Friday May 31, 2024		
08:30	Final exam	
11:30	Departure	
Notes:		
1.	There are 30-minute breaks between lectures	
2.	Lunch is served at 12h00	
3.	Dinner is served at 19h00, except on the first nice day of the week when a BBQ will be served outside.	
	1 hour LAPW basis set and show how one does the calculation with it	
	1 hour demonstration on code	