

International summer school on Computational Quantum Materials 2018

Monday May 28

08:15	P. Fournier, 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	Reza Nourafkan	Correlations in electronic structure and their signatures
11:30	X. Gonze	Abinit code, part 1
12:00	Lunch	
14:00	Poster Session	
15:00	M. Côté, X. Gonze, F. Brunival	Hands-on training: Abinit #1
16:00	M. Côté, X. Gonze, F. Brunival	Hands-on training: Abinit #1
17:00	Break	
17:30	A.-M. Tremblay	Many-Body refresher: Second quantization
18:15	A.-M. Tremblay	Many-Body refresher: Hubbard model, Evolution operators, Green functions
19:00	Dinner	

Tuesday May 29

08:30	A.-M. Tremblay	Many-Body Refresher: Spectral weight, Self-Energy
10:00	Break	
10:30	A.-M. Tremblay	Many-Body refresher: Coherent state functional integral, Anderson impurity
12:00	Lunch	
14:00	Poster Session	
15:30	X. Gonze	Abinit code, part 2
16:15	M. Côté, X. Gonze, F. Brunival	Hands-on training: Abinit #2
17:00	Break	
17:30	M. Côté, X. Gonze, F. Brunival	Hands-on training: Abinit #2
19:00	Dinner	

Wednesday May 30

08:30	A.-M. Tremblay	Many-Body Refresher: Source fields, Luttinger Ward, GW
10:00	Break	
10:30	F. Bruneval	GW method for abinit
12:00	Lunch	
15:30	M. Côté, X. Gonze, F. Brunival	Hands-on training: Abinit #3
17:00	Break	
17:30	M. Côté, X. Gonze, F. Brunival	Hands-on training: Abinit #3
19:00	Dinner	

Thursday May 31

08:30	D. Sénéchal	Dynamical Mean-Field Theory (DMFT)
10:00	Break	
10:30	A. Del Maestro	Introduction to Monte Carlo methods, Ergodicity, Detailed balance, biased sampling, variance estimate.
12:00	Lunch	
14:00	O. Parcollet	Model Hamiltonians, Introduction to TRIQS
15:30	O. Parcollet, M. Ferrero	Hands-on training: TRIQS #1 Green functions
17:00	Break	
17:30	O. Parcollet, M. Ferrero	Hands-on training: TRIQS #1 Green functions
19:00	Dinner	

Friday June 1

08:30	M. Ferrero	Continuous-time Quantum Monte Carlo (strong coupling) / (weak coupling)
10:00	Break	
10:30	A.-M. Tremblay	Many-Body Refresher: TPSC
11:15	A. Del Maestro	Entanglement in many-body systems
12:00	Lunch	
15:30	O. Parcollet, M. Ferrero	Hands-on training: TRIQS #2 IPT, CT-HYB, one band two patches
17:00	Break	
15:30	O. Parcollet, M. Ferrero	Hands-on training: TRIQS #2 IPT, CT-HYB, one band two patches
19:00	Dinner	

Monday June 4

08:30	P. Werner	Non-equilibrium problems in DMFT
10:00	Break	
10:30	P. Werner	Non-equilibrium problems in DMFT
11:15	D. Bergeron	Analytic continuation
12:00	Lunch	
14:00	O. Parcollet, M. Ferrero	Hands-on training: TRIQS #3 CT-INT, Lindhard, TPSC,
15:30	Break	
16:00	O. Parcollet, M. Ferrero	Hands-on training: TRIQS #3 CT-INT, Lindhard, TPSC,
17:30	Coffee break & free time	
19:00	Dinner	

Tuesday June 5

08:30	Michel Côté	Electron-phonon interactions
09:30	G. Kotliar	Successes and challenges in the electronic structure of correlated materials: towards theoretical spectroscopy and materials design
10:15	Break	
10:45	K. Haule	Projectors in all-electron codes
11:45	Lunch	
15:15	Bernard Amadon	Projectors in plane-wave codes
16:15	M. Côté, B. Amadon	Hands-on training: Abinit + TRIQS DMFT + DFT
17:00	Break	
17:30	M. Côté, B. Amadon	Hands-on training: Abinit + TRIQS DMFT + DFT
19:00	Dinner	

Wednesday June 6

08:30	K. Haule	Introduction to the DMFT-LAPW code I
10:00	Break	
10:30	Lucian Pascut	Wien2k tutorial
12:00	Lunch	
14:30	K. Haule	Introduction and DMFT-LAPW hands-on training #1
15:30	K. Haule	DMFT-LAPW hands-on training #2
17:00		
17:30	K. Haule	DMFT-LAPW hands-on training #2
19:00	Dinner	

Thursday June 7

08:30	A. L. Kutepov	Introduction to the features of the LAPW MBPT code
10:00	Break	
10:30	A. L. Kutepov	A hands-on training on the use of the LAPW MBPT code
12:00	Lunch	
15:30	Sangkook Choi	Introduction to GW+DMFT
17:00	Break	
17:30	Sangkook Choi	Hands-on training on GW + DMFT
19:00	Dinner	

Friday June 8

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.