ISSP International Workshop and Symposium on

Foundations and Applications of the Density Functional Theory

Workshop Program :

Place : Seminor Room #A615 ISSP 6th Floor

Week 1 (19–20 July)

	Speaker		Topic/Abstract
July 19 Thr.	Michele Casula	10:30–11:00	Introduction to the variational and diffusion Monte Carlo methods
	Michele Casula	11:30–12:30	Non local pseudopotentials in the diffusion Monte Carlo framework
July 20 Fri.	Jindrich Kolorenc	14:00–15:00	Diffusion Monte Carlo simulations of crystalline FeO under pressure

Week 2 (23–27 July)

	Speaker		Topic/Abstract
July 23 Mon.	Giulia Galli	11:00–12:00	First principle simulations of water in confined and compressed states
	Francois Gygi	14:00–15:00	Implementation of First-Principles Molecular Dynamics on Large-Scale Computers
July 24 Tue.	Giulia Galli	11:00–12:00	Quantum simulations of the structure and electronic peoperties of water
	Tadashi Ogitsu	14:00–15:00	First-principles studies of materials under extreme conditions
July 25 Wed.	Ferdi Aryasetiawan	11:00–12:00	Merging first-principles and model approaches
	Hisazumi Akai	14:00–15:00	Green's function method and its application to first-principles calculation of electric transport phenomena
July 26 Thu.	Osamu Sugino	11:00–12:00	Chemical reactions: on the Born-Oppenheimer surface and beyond
	Takeo Fujiwara	14:00–15:00	Large-scale electronic structure calculation theory and its application
July 27 Fri.	Igor Solovyev	11:00–12:00	LDA+U: fundamentals, open questions, and recent developments
	Sergey Savrasov	14:00–15:00	From LDA+U to LDA+DMFT

Week 3 (30–31 July)

	Speaker		Topic/Abstract
July 30 Mon.	Roberto Car	11:00–12:00	Dipolar correlations in water from ab-initio MD
	Annabella Selloni	14:00–15:00	The surface science of TiO_2: Insights from first-principles simulations
	Ryo Maezono	17:00–18:00	Pseudo potential QMC calculations of Porphyrin complexes
July 31 Tue.	Kieron Burke	11:00–12:00	Fundamentals of TDDFT
	John Dobson	14:00–15:00	Dispersion (van der Waals) forces and Density Functional Theory
	Ryotaro Arita	17:00–18:00	Methods for electronic structure calculations with dynamical mean field theory: An overview and recent developments

Week 4 (6–10 August)

	Speaker		Topic/Abstract
August 6 Mon.	Shinji Tsuneyuki	11:00–12:00	Transcorrelated method: another possible way towards electronic structure calculation of solids
	Roberto Car	14:00–15:00	Theory and simulation of transport at the nanoscale
August 7 Tue.	Eberhard K.U. Gross	11:00–12:00	Time-dependence in quantum transport through nanostructures
	Yasutami Takada	14:00–15:00	The electron self-energy in the Green's-function approach: Beyond the GW approximation
August 8 Wed.	Andreas Savin	11:00–12:00	Using wave functions and DFT
	Kimihiko Hirao	14:00–15:00	Molecular Theory for Large Systems
August 9 Thr.	Kieron Burke	11:00–12:00	Applications of TDDFT
	Eberhard K.U. Gross	14:00–15:00	TDDFT beyond the linear regime: Analysis and optimal control of electron dynamics
August 10 Fri.	Eberhard K.U. Gross	11:00–12:00	Degeneracies, orbital currents and non-collinear magnetism: How far can we get with current-density functional theory and orbital functionals