ISSP International Workshop and Symposium on

Foundations and Applications of the Density Functional Theory

Symposium Program:

Place : Main Lecture Hall #A632 ISSP 6th Floor

	August 1 (Wed.)	August 2 (Thr.)	August 3 (Fri.)
9:10	**Opening**		
9:30	Y. Takada (ISSP) **Eberhard K.U. Gross:** How to predict the critical temperature of superconductors: A density functional perspective	S. Tsuneyuki (U.Tokyo) **John Dobson:** Unusual Aspects of Dispersion Forces in Nanostructures	T. Fujiwara (U.Tokyo) **Igor Solovyev:** Combining DFT and many-body methods to understand correlated materials
10:00	**Kazuhiro Yabana:** Simulation for electron dynamics in solid under intense laser pulse	**Kieron Burke:** PBEsol, a generalized gradient approximation for solids and their surfaces	**Takashi Miyake:** Wannier function approach to electronic excitation spectra
10:30	**Arkady Krashennikov:** Simulations of irradiation-induced effects in carbon nanostructures	**Kouichi Kusakabe:** Multi-reference density functional theory for Mott's insulators and electron-electron interaction mediated superconductivity	**Shinji Tsuneyuki:** A wave-function approach to solids
11:00	Coffee break	Coffee break	Coffee break
11:30	T. Miyake (AIST) **Hisazumi Akai:** Exact Exchange Method Applied to Diluted Magnetic Semiconductors	J. Dobson (Griffis U) **Masahiko Higuchi:** Extended constrained-search theory and its applications	I. Solovyev (NIMS) **Ryotaro Arita:** First-principles scheme for strongly correlated electron systems with maximally localized Wannier functions: Application to black sodalite
12:00	**Takeo Fujiwara:** First Principles Electronic Structure Calculations for Strongly Correlated Systems	**Vladimir Nazarov:** Nonlocal exchange-correlation kernel from time-dependent current density functional theory: Application to the stopping power of an electron liquid	**Hideaki Maebashi:** Pseudo-quantum criticality in electron liquids exhibited in expanded alkali metals
12:30	**Sergey Savrasov:** Predictive Capabilities for Strongly Correlated Systems: Spectral Density Functional Theory and its Applications	Lunch	Lunch
13:00	Lunch		

14:00	Lunch	K. Burke (UCIrvine) **Roberto Car:** The hydrophobic effect in water: suprises from ab-initio MD	R. Maezono (JAIST) **Shigenori Tanaka:** Biomolecular calculations based on electron-correlated fragment molecular orbital methods
14:30	O. Sugino (ISSP) **Giulia Galli:** Recent progress in the description of excited state properties of liquids and nanostructures	**Kenji Hirose:** Quantum Transport Calculations through Molecules and Carbon Nanotubes	**Yutaka Imamura:** Time-dependent density functional theory for core excited states
15:00	**Minoru Otani:** First principles description of electrochemical reactions at water/Pt(111) interface	**Angelica Zacarias:** Density Matrix Functional Theory for Molecules and Solids	**Closing** (-15:10)
15:30	**Yoshitaka Tateyama:** Density-functional constrained molecular dynamics energy gap (DF-CMD-EG) method for free energy calculation of chemical reaction coupled to electron transfer	EKU Gross (FU Berlin) **Annabella Selloni:** Surface defects and doping in TiO_2	
16:00	Coffee break	Coffee break	
16:30	G. Galli (UCDavis) **Tsuyoshi Miyazaki:** Developments and applications of a linear-scaling DFT code CONQUEST	**Takao Tsuneda:** Long-range corrected TDDFT and its applications	
17:00	**Tadashi Ogitsu:** Ab-initio study of the ground state structure of elemental boron	**Chunping Hu:** Formal derivation of nonadiabatic couplings from time-dependent density functional theory and the extension within modified linear response	
17:15		Y. Tateyama (NIMS) **Kenji Shiraishi:** How can first principles calculations give large contributions to industries?	
17:30	**Francois Gygi:** Computation of Maximally Localized Wannier Functions and Compact Representations of Kohn-Sham Invariant Subspaces		
17:45			
18:00	**Yoshihide Yoshimoto:** Extended multicanonical method combined with thermodynamically optimized potential	**Shigeo Maruyama:** Exciton transition energy in photoluminescence of single-walled carbon nanotubes	
18:15	Y. Yoshimoto (ISSP) H. Maebashi (ISSP) Poster	Banquet	

chairman