Interdisciplinary Symposium on Modern Density Functional Theory

Monday 19 June 2017 - Friday 23 June 2017
Okochi Hall, RIKEN (Wako campus)

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Program

(Each keynote talk is composed of two 35-min parts and a 5-min break in between.)

June 19 (Monday)		
09:15-09:30	**Opening Session**	
Chair: S. Tsuneyuki		
09:30-10:45	Describing quantum phases of matter and their dynamics within density functional theory and time-dependent density functional theory	E.K.U. Gross
10:45-11:15	*Coffee break*	
11:15-11:45	The role of tensor force in heavy-ion fusion dynamics	L. Guo
11:45-12:15	Linear scaling solvers for density functional theory calculations	W. Dawson
	Lunch	
Chair: G. Colo		
13:30-14:45	Low-order scaling methods in density functional theories	T. Ozaki
14:45-15:15	*Coffee break*	
Chair: K. Burke		
15:15-16:30	Covariant density functional theory for nuclear structure	J. Meng
16:30-16:45	Exact time-dependent Kohn-Sham potentials in electron-scattering processes	Y. Suzuki
16:45-17:00	Maxwell+TDDFT multiscale method for light-matter interaction: Light propagation in the microscopic semiconducting crystal	M. Uemoto
17:00-17:15	Finite amplitude method for triaxially deformed superfluid nuclei	K. Washiyama
17:15-17:30	Effect of stacking interactions and conformation on polymer polarizability	K. Moorthi
18:30	***Reception Party @ Hirosawa Club***	

June 20 (Tuesday)		
Chair: J. Meng		
09:30-10:45	Basics of electron structure DFT in chemistry, condensed-matter, and materials science: From the very fundamental to the very latest (machine-learning)	K. Burke

10:45-11:15	*Symposium Photo & Coffee break*	
11:15-11:45	Large-scale first-principles electronic structure calculations in Petascale and Exascale supercomputers: A real-space density functional theory code	J. Iwata
11:45-12:15	Covariant density functional theory with Fock terms—role of the non-local Fock terms	W.H. Long
	Lunch	
Chair: T. Tsuneda		
13:30-14:45	DFT versus many-body perturbation theory for nuclear structure	G. Colo
14:45-15:15	*Coffee break*	
Chair: H.Z. Liang		
15:15-15:30	Improving usability of DFT codes by using GUI software C-Tools	K. Yoshizawa
15:30-15:45	A novel method to predict densities of amorphous materials from first-principles calculations	Y. Furukawa
15:45-16:00	Spin and spin-isospin responses in $N=Z$ nuclei and isoscalar pairing correlations	H. Sagawa
16:00-16:15	Spin-isospin responses in low-energy	K. Yoshida
16:15-16:30	Tensor effects on the isospin excitation with random phase approximation based on relativistic Hartree-Fock approach	Z.H. Wang
16:30-16:45	Band unfolding calculations compared with ARPES experiments: Examples of Ni1/3TiS2 and twisted-bilayer graphene	Y. Matsushita

June 21 (Wednesday)		
Chair: E.K.U. Gross		
09:30-10:45	From density functional to many-body Green's function and beyond	O. Sugino
10:45-11:15	*Coffee break*	
11:15-11:45	Nuclear Gamow-Teller excitation and beta decay study within modern density functional theory	Y.F. Niu
11:45-12:15	Development of two-component relativistic time-dependent density functional theory for Molecular Properties	M. Kamiya
Free afternoon		

June 22 (Thursday)		
Chair: T. Otsuka		
09:30-10:45	Quantized TDDFT dynamics	T. Nakatsukasa
10:45-11:15	*Coffee break*	
11:15-11:45	A quantum dynamics descriptor for exploring a mechanism of light-driven electron migration in molecular aggregated system	T. Yonehara
11:45-12:15	Quantifying the impact of Plasmon and Paramagnon effects in "conventional" superconductors from the first principles	R. Akashi
	Lunch	

Chair: O. Sugino		
13:30-14:45	Quantum phase transition and quantum self-organization in nuclear to mesoscopic many-body systems	T. Otsuka
14:45-15:15	*Coffee break*	
Chair: W. Weise		
15:15-16:30	Long-range exchange interactions in DFT and their significance in chemical reactions	T. Tsuneda
16:30-16:45	Anderson-Bogoliubov phonon in inner crust of neutron stars	T. Inakura
16:45-17:00	A unified description for strange quark matter objects	C.J. Xia
17:00-17:15	Momentum-space quasiparticle RPA calculation with Skyrme energy density functional for rotating weakly-bound nuclei	M. Yamagami
17:15-17:30	Cluster multipole theory for anomalous Hall effect in antiferromagnets	M. Suzuki

June 23 (Friday)		
Chair: T. Nakajima		
09:30-10:45	From low-energy QCD to nuclear physics and energy density functionals	W. Weise
10:45-11:15	*Coffee break*	
11:15-11:45	Computational materials database toward discovering novel semiconductors	Y. Kumagai
11:45-12:15	Development of the fragment molecular orbital method combined with DFT and DFTB and applications to proteins	D. Fedorov
12:15-12:20	**Closing Session**	