THURSDAY MORNING * Room 29D
David Reichman, Presiding

8:00 (615). Electron dynamics calculations of ultrafast energy transfer processes in quantum dots. A. Bande


9:10 (617). Attosecond electronic band dynamics. S.R. Leone

9:55 INTERMISSION


THURSDAY AFTERNOON * Room 29C
Dominika Zgid, Presiding

1:30 (667). On couplings and excimers: Lessons from studies of singlet fission in covalently linked dimers. X. Feng, A. Krylov

2:15 (668). Accurate excitation energies for systems with near-degeneracies. D. Lambrecht


3:25 INTERMISSION


4:10 (671). Quantum Monte Carlo for excited states in complex environments. C. Filippi

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251st National ACS Meeting
Division of Physical Chemistry

Towards Predictive Calculations in Strongly Correlated Molecules & Materials

Timothy C. Berkelbach
Eric Neuscamman
Organizers

March 13-16, 2016
San Diego Convention Center
ROOMS 29D / 30A / 29C
SUNDAY MORNING  *  Room 29D  
Sandeepr Sharma, Presiding

8:00 (43). Applications of density matrix renormalization group algorithm-based multireference correlation theories. Y. Kurashige
8:45 (44). Low-rank tensor approximations for many-electron wavefunctions in Hilbert space. Z. Li, G.K. Chan
9:10 (45). Active space decomposition for excited states and strongly correlated electronic structure. T. Shiozaki

9:55 INTERMISSION

11:00 (47). PySCF: A novel open-source computational tool for the electronic structure problem. Q. Sun

SUNDAY AFTERNOON  *  Room 29D  
Toru Shiozaki, Presiding

1:30 (90). Renormalization group approaches for strongly correlated electrons. F.A. Evangelista
2:15 (91). Combining density matrix renormalization group and n-electron valence perturbation theory. S. Guo, G.K. Chan
2:40 (92). Efficient multireference dynamic correlation from time-dependent perturbation theory. A. Sokolov, G. Chan
3:25 INTERMISSION

3:45 (93). Solving a challenge posed by experiment: Characterizing the ground and excited states of nickel silicide. G. Schoendorff, A. Morris, E. Hu, A.K. Wilson
4:10 (94). Recent progress in multireference dynamic correlation methods based on density matrix renormalization group. T. Yanai, M. Saitow, Y. Kurashige
4:55 (95). Non-perturbative diagrammatic calculation of ionization potential using R12-correlator operator. M. Bayne, A. Chakraborty

MONDAY MORNING  *  Room 30A  
Francesco Evangelista, Presiding

8:00 (140). Stochastic and deterministic solutions of multireference linearized coupled cluster equations. S. Sharma
8:45 (141). Efficient modeling of transition metal systems using approximate projection: development and applications. L.M. Thompson, H.P. Hratchian
9:10 (142). Novel wavefunction approaches for strongly correlated electrons. G.E. Scuseria
9:55 INTERMISSION

10:15 (143). Density functional model for nondynamic and strong correlation. J. Kong, E. Proynov
10:40 (144). Two-electron reduced density matrix methods for strongly correlated quantum systems. D.A. Mazzotti

MONDAY AFTERNOON  *  Room 29D  
Eric Neuscamman, Presiding

1:30 (188). Highly accurate fragment molecular orbital/quantum Monte Carlo method for large molecular systems. S.R. Pruitt, A. Benali, D. Fedorov
3:25 INTERMISSION

3:45 (191). Obtaining trial wavefunctions on the cheap: A stochastic approach to multietdeterminant wavefunctions in auxiliary field quantum Monte Carlo. B.M. Rubenstein, M. Morales-Silva, C. Chang, E. Landinez-Borda
4:30 (192). Electron correlation in an atomic chain of gold atoms. J. Greer, T. Kelly

TUESDAY MORNING  *  Room 29D  
Timothy Berkelbach, Presiding

8:00 (245). Density matrix embedding theory: Accurate reaction paths and a second-quantized formulation for the local density of states. S. Wouters, G.K. Chan
8:45 (246). Two-dimensional embedded cluster method for accurate modeling of reactivity at oxide interfaces. A.B. Muñoz-García, J. Pascual Robledo, M. Pavone
9:55 INTERMISSION

10:15 (248). Non-equilibrium electron dynamics from a real-time extension of density matrix embedding theory. J. Kretchmer, G. Ch.

WEDNESDAY MORNING  *  Room 29D  
Troy Van Voorhis, Presiding

8:00 (306). Systematically improvable Green's function embedding methods for molecules and solids. D. Zgid
9:10 (308). Hubbard operator density functional theory for Fermion lattice models. Z. Cheng, C. Marianetti
9:55 INTERMISSION

11:00 (310). Taming the dynamical sign problem in the real time evolution of quantum impurity problems. D.R. Reichman