Thursday Morning
Macromolecular Dynamics
Bruce C. Garrett, Presiding

8:00 (569). Computationally guided design and optimization of inhibitors of macrophage migration inhibitory factor. **W.L. Jorgensen**, D.J. Cole, M.J. Robertson

8:30 (570). Multiscale characterization of macromolecular dynamics. **C. Clementi**

9:00 (571). Dynamic effects in dihydrofolate reductase catalysis. **R.K. Allemann**, L. Luk, J. Loveridge

9:30 (572). Advancing ab initio molecular dynamics via multiple-timestep methods. **R. Steele**

9:50 INTERMISSION

10:10 (573). Toward a molecular theory of early and late events in monomer to amyloid fibril formation. **J.E. Straub**

10:40 (574). Large spatiotemporal-scale quantum molecular dynamics simulations: A divide-conquer-recombine approach. **A. Nakano**, R.K. Kalia, K. Nomura, K. Shimamura, F. Shimojo, P. Vashishta

11:10 (575). Sorbate dynamics in hierarchical porous materials. **J.I. Siepmann**, P. Bai, E. Haldoupis, M. Tsapatsis

11:30 (576). Molecular dynamics simulations of ion transport in carbon nanotubes. **K.L. Shuford**, O. Samoylova, E. Calixte

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249th National ACS Meeting

Division of Physical Chemistry

Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed-Phase Systems

A Symposium in Honor of Donald Truhlar

Jiali Gao
Bruce C. Garrett
Benedetta Mennucci

ORGANIZERS

Colorado Convention Center

March 22-26, 2015

ROOM 503

Sunday Morning
Accurate Energies for Dynamics
Mark S. Gordon, Presiding

8:00 (14). Potential energy surfaces for dynamics calculations. **D.G. Truhlar**

8:30 (15). Strategies towards dynamic and non-dynamic electron correlation. **A.K. Wilson**

9:00 (16). Dissecting the effect of morphology on the rates of singlet fission: Insights from theory. **A. Krylov**

9:20 (17). Aerobic oxidation of methanol to formic acid on Au_8^-: Benchmark analysis based on completely renormalized coupled-cluster and density functional theory calculations. **P. Piecuch**, J.A. Hansen, M. Ehara

9:40 INTERMISSION

10:00 (18). Complications in potential energy surfaces for molecules involving second row elements. **T.H. Dunning**

10:30 (19). Dynamics of curved carbon π systems. **K.K. Baldridge**

11:00 (20). Mag-walking Monte Carlo and density functional theory calculations of interaction energies in ammonium halide clusters. **R.Q. Topper**, J.J. Biswakarma, V. Ciocoi

11:20 (21). Analysis of changes in bonding patterns along reaction paths in terms of molecule-intrinsic quasi-atomic orbitals. **K. Ruedenberg**, A.C. West, M.W. Schmidt, M.S. Gordon

Sunday Afternoon
Gas-Phase Kinetics and Dynamics
George C. Schatz, Presiding

1:30 (73). Mode-, bond- and stereo-selective bimolecular reactions. **K. Liu**

2:00 (74). Sudden vector projection model: Mode specificity and bond selectivity made easy. **H. Guo**

2:30 (75). Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering. **D. Babikov**

2:50 (76). Sum over histories representation for chemical kinetics. **R.T. Skodje**

3:10 INTERMISSION

3:30 (77). Cold chemistry: Quantum reactive scattering calculations of O + OH → O_2 + H and Li + LiYb → Li_2 + Yb. **B. Kendrick**

3:50 (78). Reaction dynamics on ab initio potential energy surfaces. **J.M. Bowman**, Y. Wang , Z. Homayoon, R. Conte, P. Houston

4:20 (79). Improved semiclassical tunneling. **A.F. Wagner**

4:50 (80). Alkyl CH stretch vibrations as a probe local environment. **E.L. Sibert**, D.P. Tabor, N. Kidwell, J.C. Dean, T.S. Zwier

Monday Morning
Enzyme Kinetics and Dynamics
Sharon Hammes-Schiffer, Presiding

8:00 (124). Tunneling and the role of barrier width in enzymatic C-H activation. **J.P. Klinman**

8:30 (125). Theoretical studies of enzymatic reactions. **W. Thiel**

9:00 (126). BioEFP: Effective fragment potential method for biological systems. **L.V. Slipchenko**

9:20 (127). Quantum mechanical/molecular mechanical simulations of the hydride transfer reactions in quinone reductase 2. **C.R. Reinhardt**, S. Bhattacharyay

9:40 INTERMISSION

10:00 (128). QM/MM excited state dynamics of complex systems. **U. Roethlisberger**

10:30 (129). Understanding metalloenzyme catalysis with QM/MM free energy simulations. **Q. Cui**

11:00 (130). Adaptive-partitioning QM/MM dynamics simulations of proton transfer. S. Pezeshki, **H. Lin**

11:20 (131). Functional mode electron transfer theory. **H. Chen**

Monday Afternoon
Catalysis
Charles T. Campbell, Presiding

1:30 (179). Silica thin films: From crystals to glass in 2D. **H. Freund**

2:00 (180). Doped metal clusters on oxides: Rationalization and design through the prism of chemical bonding. **A. Alexandrova**

2:30 (181). Some recent developments in saddle point finding methods: Gradient squared minimization, solid state transitions, and temperature accelerated adaptive kinetic Monte Carlo. **G.A. Henkelman**

3:00 (182). Catalysis with metal clusters anchored at the Zr6-based metal-organic framework NU-1000. **L. Gagliardi**, D.G. Truhlar, C.J. Cramer, J. Borycz, L. Fernandez, S. Tussupbayev

3:20 INTERMISSION

3:40 (183). New approaches to simulating biological and molecular catalysts. **T.F. Miller**

4:10 (184). Organometallic and organocatalytic reactions explored using the automated reaction route mapping method. **K. Morokuma**

4:40 (185). Hydrazine decomposition in the gas phase and on an Iridium catalyst. **M.W. Schmidt**, M.S. Gordon

5:00 (186). Density functional theory study of lithium ion battery anode materials: Ruthenium (IV) oxide, tin (IV) oxide, and tin (IV) sulfide. **B.R. Ramachandran**, A.S. Hassan, K. Moyer, T. Dixon, C.D. Wick

Wednesday Morning
Properties and Processes in Solvated Systems
Benedetta Mennucci, Presiding

8:00 (277). 25 years of SM*x* models: Quantum and classical continuum solvation. **C.J. Cramer**, D.G. Truhlar

8:30 (278). Protein aggregation, collapse, and disorder: Model systems. **B.M. Pettitt**, D. Karandur

9:00 (279). Role of dynamics in enzyme catalysis: Challenges in comparing calculations to measurements. **A. Kohen**

9:20 (280). Role of solvent structure on the rate of ion-pairing. **M.D. Baer**, C.J. Mundy, G.K. Schenter

9:40 INTERMISSION

10:00 (281). Quantum-classical path integral: A rigorous methodology. **N. Makri**

10:30 (282). Structure, properties, excited states and reactivity of complex systems in solution: Putting together the pieces. **G. Scalmani**, M.J. Frisch

11:00 (283). How reliable are calculations of absorption spectra of solvated molecules with CC theory and PCM? **M. Caricato**

11:20 (284). Continuum solvation calculations of solvatochromic shifts: Recent advances and perspectives. **A.V. Marenich**, C.J. Cramer, D.G. Truhlar, G. Scalmani, M.J. Frisch

Wednesday Afternoon
Nonadiabatic Dynamics
Xiaosong Li, Presiding

1:30 (332). Beyond the Born-Oppenheimer approximation: Construction of accurate multicomponent wave function using explicitly-correlated and projection-based methods. **A. Chakraborty**

2:00 (333). Directly correlating electronic and vibrational motions with multidimensional coherent spectroscopies. **M.H. Khalil**

2:30 (334). Approximate time-dependent diabatic states computed using a measure driven tessallation technique for use in on-the-fly quantum dynamics methods. **S.S. Iyengar**

3:00 (335). Avoiding the Born-Oppenheimer separation between electrons and protons in wavefunction and density functional theory calculations. **S. Hammes-Schiffer**

3:20 INTERMISSION

3:40 (336). Surface hopping and spectroscopy. **J.E. Subotnik**, A.S. Petit

4:10 (337). Novel approaches to nonadiabatic molecular dynamics. **O.V. Prezhdo**

4:40 (338). Time-dependent electronic and nuclear potentials that exactly capture electron-ion coupling. **N. Maitra**

5:10 (339). Time-derivative coupling scheme for accurate electronic state transition probabilities in nonadiabatic molecular dynamics. **G. Meek**, B. Levine