**POSTER SESSION A - Tuesday, July 22**

**A1. Redox properties of green fluorescent proteins and their chromophores**

Atanu Acharya, Debashree Ghosh, Anna I. Krylov

**A2. Efficient calculation of transport and dielectric properties, with application to the frequency-dependent dielectric response of a DNA oligomer**

Mithila V. Agnihotri, Si-Han Chen, Corey Beck, Sherwin J. Singer

**A3. A case study on anti-aromaticity: Structure and energetics of the methylcarboxylate cyclopropenyl anion**

Sevgi Şahin, Erdi A. Bleda, Zikri Altun, Carl Trindle

**A4. A polarizable water model developed with the adaptive force matching method**

Saieswari Amaran, Tomasz Janowski, Peter Pulay, Revati Kumar, Tom Keyes,Feng Wang

**A5. PCET in the C5H5N∙(H2O)3- Anion: An experimentally motivated theoretical study**

Kaye A. Archer, Kenneth D. Jordan, Andrew DeBlase, Tim Guasco, Mark A. Johnson

**A6. Quantum Monte Carlo study of HCP solid 4He: Searching for anisotropy in the Debye-Waller factor**

Ashleigh Barnes, Robert Hinde

**A7. Combining active-space coupled-cluster approaches with moment energy corrections via the CC(*P*;*Q*) methodology: connected triple and quadruple excitations**

Nicholas P. Bauman, Jun Shen, Piotr Piecuch

**A8. Empirical valence bond potentials for the capture of acidic gases by ionic liquids**

Lindsay R. Baxter, Daniel M. Chipman, Steven A. Corcelli

**A9. Fischer-Tropsch mechanistic pathways as elucidated by the *ab initio* nanoreactor**

Leah Isseroff Bendavid, Lee-Ping Wang, Todd Martinez

**A10. Water-like anomalies and its relationship with ordered structures**

Andressa Antonini Bertolazzo, Valeria Molinero

**A11. Modeling membrane sculpting from single proteins to mesoscale morphology changes**

Ryan Bradley, Natesan Ramakrishnan, Richard Tourdot, Ravi Radhakrishnan

**A12. Excitation energy transfer in the Peridinin-Chlorophyll *a*-protein complex modeled using configuration interaction**

William P. Bricker, Cynthia S. Lo

**A13. Assessment of amide I spectroscopic maps for a gas-phase peptide**

Joshua K. Carr, Aleksandra V. Zabuga, Santanu Roy, Thomas R. Rizzo, James L. Skinner

**A14. Diabatization methods for high accuracy treatment of spectroscopic systems**

Robin Bendiak, John F. Stanton, Robert J. Cave

**A15. Accuracy of non-equilibrium Pade-Resummation master equation approach to dissipative quantum dynamics**

Hsing-Ta Chen, David R. Reichman

**A16. Static and dynamic properties of the electrical double layer near amorphous silica**

Si-Han Chen, Hui Zhang, Ali Hassanali, Sherwin J. Singer

**A17. Embedded correlated wavefunction theory: development and application**

Jin Cheng, Florian Libisch, Emily A. Carter

**A18. Anharmonic vibrational spectroscopy calculations using local-mode coordinates**

Xiaolu Cheng, Ryan P. Steele

**A19. Quantum diffusion on a tube**

Chern Chuang, Jianshu Cao

**A20. Surface-enhanced Raman optical activity using atomistic electrodynamics-quantum mechanical models** Dhabih Chulhai and Lasse Jensen

**A21. The geometry of transition state structure in chemical reactions driven by fields oscillating in time**

Galen T Craven, Thomas Bartsch,Rigoberto Hernandez

**A22. Anharmonic vibrational Frequencies of CO2 complexed with ionic liquids**

Clyde A. Daly Jr., Steven A. Corcelli

**A23. Applications of Qauntum Monte Carlo to weakly interacting systems**

Michael Deible, Kenneth D. Jordan

**A24. Mixed quantum-classical dynamic simulation of exciton dissociation at organic interfaces**

Olivia Dinica, Peter Rossky

**A25. Thermodynamics of coarse-grained models: Reproducing atomistic volume fluctuations**

Nicholas J. H. Dunn, William G. Noid

**A26. Time-resolved spectroscopy to follow electronic motion in molecules: A study of molecular alignment**

Anthony D. Dutoi, Lorenz S. Cederbaum

**A27. Density functional calculations of an inhomogenous 4He system**

Matt Dutra, Robert Hinde

**A28. Challenges in comparing SN1 vs SN2 rates *ab initio*: the mechanism of ether-catalyzed hydroboration of alkenes**

Daniel J. S. Sandbeck, Colin M. Kuntz, Rachelle A. Mondor, John G. Ottaviano, Aravind V. Rayer, Kazi Z. Sumon, Allan L. L. East

**A29. A simple approach to the vapour pressure of bulk and nano systems**

Matias Factorovich, Valeria Molinero, Damian Scherlis

**A30. Graphical processing unit acceleration of two step methods**

B. Scott Fales

**A31.** **First principles modeling of mechanically-assisted ring opening of *gem*-dichlorocyclopropanes**

Lin Fan, Todd J. Martínez

**A32. Utilizing light for repair of light-induced DNA damages: the clever mode of action of DNA photolyases**

Shirin Faraji, Andreas Dreuw

A33. Information in a rate coefficient: When are rate coefficients constant?

Shane W. Flynn, Helen C. Zhao, Jason R. Green

**A34. Electrochemical solvent reorganization energies in the framework of the polarizable continuum model**

Soumya Ghosh, Samantha Horvath, Alexander V. Soudackov,Sharon Hammes-Schiffer

**A35. A parallel multistate framework for non-equilibrium reaction dynamics in strongly interacting organic solvents: F abstraction reactions in *d*-acetonitrile**

David R. Glowacki, Andrew J. Orr-Ewing, Jeremy N. Harvey

**A36. Attenuated second order Møller-Plesset perturbation theory: correcting finite basis set errors and infinite basis set inaccuracies**

Matthew Goldey, Martin Head-Gordon

**A37. QM/MM nonadiabatic dynamics of photoinduced proton-coupled electron transfer in solution**

Puja Goyal, Christine A. Schwerdtfeger, Alexander V. Soudackov, Sharon Hammes-Schiffer

**A38. Theoretical vibrational one- and two-dimensional sum-frequency generation spectroscopy of water near lipid and surfactant monolayer interfaces**

Scott M. Gruenbaum, Santanu Roy, James L. Skinner

**A39. Dyson orbitals within EOM-CC formalism**

Anastasia O. Gunina, Anna I. Krylov

**A40. Bottom-up insight into the morphology, spectroscopy, and photophysics of polythiophene**

Ryan Haws, Peter Rossky

**A41. Imaginary-time nonuniform mesh method for solving the multidimensional Schroedinger equation**

Alberto Hernando De Castro, Jiri Vanicek

**A42. Insight into the structures and electronics of water oxidation**

Jonathan Herr

**A43. The moving-oomain QM/MM method for self-consistent structural refinement: Characterization of the Oxytricha nova G-quadruplex**

Junming Ho, Michael B. Newcomer, Jose A. Gascon, Victor S. Batista

**A44. Reduced scaling in electronic structure theory via tensor hypercontraction**

Edward G. Hohenstein, Todd J. Martinez

**A45. On the transferability of three water models developed by adaptive force fitting (AFF)**

Hongyi Hu, Zhonghua Ma, Feng Wang

**A46. Mechanochemistry of persistent plasmid movement**

Longhua Hu, Jian Liu

**A47. Simulating nonlinear optical spectroscopies with a time-dependent density functional approach** Zhongwei Hu and Lasse Jensen

**A48. Molecular nanoplasmonics:QM/EM for hot carrier transport and surface enhanced raman scattering**

Ying Huang, Lingyi Meng, Chiyung Yam, Prof. Guanhua Chen

**A49. Development of a new coarse-grained model of organic molecules – ketones, mono and di-carboxylic acids**

Ar9a Hudait, Valeria Molinero

**A50. Mechanistic insights for hydrogen evolution catalyzed by nickel-iron and iron-iron hydrogenase models**

Mioy T. Huynh, David Schilter, Thomas B. Rauchfuss, Sharon Hammes-Schiffer

**A51. Using nonlinear dimensionality reduction techniques to characterize reaction pathways**

Sofia Izmailov, Todd J. Martinez

**A52. Structural disorder in conjugated polymers**

Nicholas E. Jackson, Brett M. Savoie, Kevin L. Kohlstedt, Monica Olvera de la Cruz, George C. Schatz, Lin X. Chen, Mark A. Ratner

**A53. Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks**

Thomas-C. Jagau,Dmitry Zuev, Ksenia B. Bravaya, Anna I. Krylov

**A54. Computing rates of symmetric proton tunneling using semiclassical methods**

Amber Jain, Edwin L. Sibert III

**A55. Development of large-scale first-principles Ehrenfest dynamics and its application to electronic excitation by proton radiation**

Kyle Reeves, Andre Schleife, Alfredo Correa, Yosuke Kanai

**A56. A scaled-ionic-charge simulation model that reproduces enhanced and suppressed water diffusion in aqueous salt solutions**

Zachary R. Kann, James L. Skinner

**A57. Atomic-level characterization of the hydrophobicity of the GroE chaperonin identifies two interfacial salt bridges that may be influential in the reversible binding of GroES**

Lauren H. Kapcha, Chandrajit L. Bajaj, Peter J. Rossky

**A58. Accelerating quantum instanton calculations of kinetic isotope effects**

Konstantin Karandashev, Jiri Vanicek

**A59. Combining quantum-classical dynamics techniques with master equation methods: Exploiting complementary time-scales.**

Aaron Kelly**,** Thomas E. Markland

**A60. Atomistic simulations of chemically heterogeneous aluminum−gallium interfaces**

Jesse L. Kern, Brian B. Laird

**A61. Efficient linear-scaling density functional theory for molecular systems**

Rustam Z. Khaliullin, Joost VandeVondele, Juerg Hutter

**A62. Non-BO calculations of rovibrational states of diatomic molecules**

Nikita Kirnosov, Ludwik Adamowicz

**A63. Computing absorption spectra with GPU accelerated tensor hypercontraction EOM-CC2**

Sara Kokkila, Edward Hohenstein, Robert Parrish, Todd Martínez

**A64. Excited state properties of flexible organic chromophores: Quantifying intermolecular interactions and dynamical effects**

Tim Kowalczyk, Cristopher Camacho, Stephan Irle

**A65. The ring-opening of the cyclopropyl radical: Dynamics and isotope effects on a system with a reaction path bifurcation**

Zeb Kramer, Barry K. Carpenter, Stephen Wiggins, Gregory S. Ezra

**A66. Direct simulation of proton-coupled electron transfer reaction dynamics and mechanisms**

Joshua S. Kretchmer, Thomas F. Miller, III

**A67. Tuning the dimensionality of water and solute networks in binary solutions of water and simple isotropic solutes**

Abhinaw Kumar, Andrew Nguyen, Valeria Molinero

**A68. Perturbative frozen natural orbital EOM-IP-CCSD method**

Alexander A. Kunitsa, Ksenia B. Bravaya

**A69. Shielding of dynamic electric field by single-wall carbon nanotubes**

YanHo Kwok, ChiYung Yam, GuanHua Chen

**A70. Accurate intermolecular interaction energy components for many-body systems**

Ka Un Lao, John M. Herbert

A71. Self-consistent Perdew-Zunger self-interaction correction to density-functional theory

Susi Lehtola, Hannes Jónsson

**A72. New insights into the mechanism of Py-catalyzed CO2 reduction on GaP electrodes**

Martina Lessio*,* Emily A. Carter

**A73. Pairwise-additive force field for ions from adaptive force matching**

Jicun Li and Feng Wang

**A74. Theoretical investigation of photocatalysis using of constrained density functional theory**

Yao Li, Dominika Zgid

**A75. The role of large amplitude motions in the H3+ + H2 → H5+ → H3+ + H2 reaction**

Zhou Lin, Anne B. McCoy

**A76. Polarizable continuum solvation models on graphical processing units**

Fang Liu, Todd J. Martínez

**A77. Vibrational relaxation and spectral lineshape of dilute HOD in Ice Ih**

Hanchao Liu, Yimin Wang, Joel M. Bowman

**A78. Coarse-graining of popular atomistic water models to monoatomic anisotropic ones using the relative entropy minimization**

Jibao Lu, Yuqing Qiu, Riccardo Baron, Valeria Molinero

**POSTER SESSION B – Wednesday, July 23**

**B1. The nature of the asymmetry in the hydrogen-bond networks of hexagonal ice and liquid water**

Thomas D. Kuehne, Rustam Z. Khaliullin

**B2. Parameterization of DFTB3/3OB for phosphorus and magnesium and QM/MM free energy simulations to explore ATP hydrolysis in myosin**

Xiya Lu, Qiang Cui

**B3. Heterogeneous nucleation of ice on carbon surfaces**

Laura Lupi, Valeria Molinero

**B4. Electronic excitations of silver nanoclusters: A study using time dependent density functional theory**

Lindsey R. Madison, Mark A. Ratner, George C. Schatz

**B5. Rigorous quantum calculations and many-body potential energy surfaces: Applications to pure mixed HCl and water clusters**

John S. Mancini*,* Joel M. Bowman

**B6. Dispersion forces on nuclei of molecules within a dielectric framework**

Anirban Mandal, Katharine L. C. Hunt

**B7. Effect of alkyl spacer length on the phase behavior of Gemini dicarboxylate surfactants**

Sriteja Mantha, Dominic Perroni, Mahesh Mahanthappa, Arun Yethiraj

**B8. Theoretically computed Pourbaix diagrams for the design of efficient CO2 reduction co-catalysts**

Aude Marjolin, Mitchell C. Groenenboom, Karthikeyan Saravanan, Yaqun Zhu, John Keith

**B9. Exact system-bath model dynamics as an approximation to electron transfer dynamics**

Michael G. Mavros, Troy Van Voorhis

**B10. Ab initio force field development for complex materials.**

Jesse McDaniel

**B11. Intrinsic effects of glycosylation on protein folding and stability**

Sean McHugh, Yu-Shan Lin

**B12. Improved evaluation of the time-derivative coupling for accurate electronic state transition probabilities**

Garrett A. Meek, Benjamin G. Levine

**B13. A protocol based on petascale electronic structure calculations for obtaining accurate energetics of (H2O)*n*: application to *n* = 2 – 25**

Evangelos Miliordos,Edoardo Aprà*,* Sotiris S. Xantheas

**B14. Probing ultrafast molecular dynamics of electronically excited thymine with Auger decay**

S. Miyabe, T. J. Martinez

**B15. Reduced density matrix hybrid approach: Extending the applicability of the Redfield Equation**

Andres Montoya-Castillo, Timothy C. Berkelbach, David R. Reichman

**B16. A discrete interaction model/quantum mechanical method for simulating optical properties of molecules on metal surfaces** Justin E Moore, Seth M Morton, Lasse Jensen

**B17. The structure of ice-clathrate interface**

Andrew H. Nguyen,Matthew A. Koc, Tricia D. Shepherd, Valeria Molinero

**B18. Diabatization of electronic excited states in an atom-centered bath**

Triet S. Nguyen, Ravindra Nanguneri, Thomas Markovich, Samuel Blau, John A. Parkhill

**B19. Contribution of van der Waals interactions to the stability of polypeptide chains in helical conformations**

Jorge Nochebuena, Beatriz Ramírez, Joel Ireta

**B20. Hammett relationships in electronic excited states: An extrathermodynamic approach to complete active space valence-bond theory**

Seth Olsen

**B21. Understanding and predicting protein function with computed electrostatic and chemical properties**

Mary Jo Ondrechen

**B22. Implementation of exact and approximate methods for nonadiabatic quantum molecular dynamics induced by the interaction with the electromagnetic field**

Aurélien Patoz, Jiri Vanicek

**B23. Molecular properties from density functional theory: An *ab initio* approach to design “new generation” inhibitors**

Niladri Patra, Heather J. Kulik

**B24. How to calculate spectra using fewest switches surface hopping trajectories: A simple generalization of ground-state Kubo theory**

Andrew S. Petit, Joseph E. Subotnik

**B25. Selectivity and dynamics of surface-bound heterogeneous catalysts**

William C. Pfalzgraff, Aaron Kelly, Thomas E. Markland

**B26. Modeling the mechanical sensitivity of chemical reaction rates**

Nikolay V. Plotnikov, Todd J. Martinez

**B27. Comparison of DFT functionals for the description of Ruthenium terpyridine complexes**

Julia Preiß, Benjamin Dietzek, Todd Martínez, Martin Presselt

**B28. Vibrational frequencies of isolated and solvated *N*-methylacetamide: Application of fragmentation method**

Chen Qu, Joel M. Bowman

**B29. Ice nucleation and phase segregation in water/alkane mixtures and at interface**

Yuqing Qiu, Valeria Molinero

**B30. Improving the accuracy of coarse-grained models: mappings, intramolecular conformations, and many-body correlations**

Joseph F. Rudzinski, Will G. Noid

**B31. Quantum chemical engineering: Can we use quantum tunneling to improve gas separations?**

Joshua Schrier

**B32. Rank-reduced full configuration interaction**

Nick F. Settje, Todd J. Martínez

**B33. Recent progress in the electron-attached, ionized, and active-space equation-of-motion coupled-cluster methodologies**

Jun Shen, Piotr Piecuch

**B34. Mechanism of DNA binding to amorphous silica**

Bobo Shi, Ali Hassanali, Yun Kyung Shin, Sherwin Singer

**B35. Phase space approach to solving the time-independent Schrodinger equation: Thinking inside the box**

Asaf Shimshovitz, David Tannor

**B36. Aqueous interfacial structure imposed by hydrogen bonding network**

Sucheol Shin, Adam P. Willard

**B37. Excited state dynamics of oxygen-containing defects on the silicon surface**

Yinan Shu, Benjamin G. Levine

**B38. Conditional convergence hiding in plain sight: summation order for the Coulomb-potential bipolar expansion makes a difference when the charge distributions overlap**

Harris J. Silverstone

**B39. Development of non-Born-Oppenheimer electronic structure methods for the quantum treatment of protons** Andrew Sirjoosingh, Sharon Hammes-Schiffer

**B40. A framework for massively parallel atomistic dynamics simulation of photosynthetic energy transfer: An empirical exciton approach**

Aaron Sisto, David Glowacki, Todd Martinez

**B41. Growth of ice and its prevention by antifreeze proteins** Diana Slough, Yu-Shan Lin

**B42. CO2 adsorption on carbon nanotubes: coupled-cluster benchmarks for model systems and selection of an optimal DFT variant**

Daniel G. A. Smith, Konrad Patkowski

**B43. Investigating excited state proton transfer in green fluorescent protein**

James W. Snyder Jr., Todd J. Martinez

**B44. Entropy-driven molecular separations in 2D-nanoporous materials, with application to high-performance**

**paraffin/olefin membrane separations**

Kylen Solvik, Joshua Schrier

**B45. Improving coarse grained model for water in macromolecular systems with soft interaction potentials** Chang Yun Son, Qiang Cui, Arun Yethiraj

**B46. Can guest occupancy in double clathrate hydrates be tuned through control of the growth conditions?**

Bin Song, Andrew H. Nguyen, Valeria Molinero

**B47. Molecular dynamics with GPU accelerated tensor hypercontraction**

Chenchen Song, Todd J. Martínez

**B48. A greener path to ethylene epoxidation in doped mesoporous silica matrices**

Krista G. Steenbergen, Jesse L. Kern, Pansy D. Patel, Ward H. Thompson, Brian B. Laird

**B49. Relation of exact Gaussian basis methods to the dephasing representation: Theory and application to time-resolved electronic spectra**

M. Šulc,H. Hernández,Todd J. Martínez, J. Vaníček

**B50. Solute-pump/solvent-probe spectroscopy and preferential solvation dynamics**

Xiang Sun

**B51. Zinc oxide nanoparticle formation using a reactive force field**

Craig J. Tainter, George C. Schatz

**B52. Fundamental sspects of the recoupled pair bond model and through-pair interactions: Generalized valence bond analysis of NX, F(NX) and H(NX), X=O, S**

Tyler Y. Takeshita, Lu T. Xu, Beth A. Lindquist,Thom H. Dunning Jr.

**B53. *Ab initio* reaction kinetics of hydrogen abstraction from methyl acetate and subsequent unimolecular decomposition reactions of radicals** Ting Tan, Emily A. Carter

**B54. Analyses of proton transport in water from ab initio molecular dynamics simulations**

Ying-Lung Steve Tse, Christopher Knight, Gregory Voth

**B55. Analytical gradients of constrained density functional theory-configuration interaction**

Takashi Tsuchimochi, Benjamin Kaduk, Troy Van Voorhis

B56. Nonadiabatic spin-forbidden binding of H2 to the active site of [NiFe]-hydrogenase

Danil S. Kaliakin, Ryan R. Zaari, Sergey A. Varganov

**B57. Computational modeling and design of nonbiological protein assemblies**

Christopher D. Von Bargen, Matthew J. Eibling, Christopher M. MacDermaid, Christopher J. Lanci, J. Kent Blasie, Michael J. Therien, Jeffery G. Saven

**B58. Predictions of coarse-grained model sensitivity to underlying fine-grained parameters using single point formulae**

Jacob W. Wagner, James F. Dama, Gregory A. Voth

**B59. Discovering chemistry with an *ab initio* nanoreactor**

Lee-Ping Wang, Alexey Titov, Robert McGibbon, Fang Liu, Vijay S. Pande, Todd J. Martínez

**B60. Quantum delocalization of protons in the ketosteroid isomerase active site**

Lu Wang, Stephen D. Fried, Yufan Wu, Steve G. Boxer, Thomas E. Markland

**B61. SMPBE:  An improved mean-field electrostatics method for biomolecules**  
Nuo Wang, Peter Kekenes-Huskey, Shenggao Zhou, Bo Li, J. Andrew McCammon

**B62. Mode-specific tunneling in the unimolecular dissociation of *cis-*HOCO and HCO**

Xiaohong Wang, Joel M. Bowman

**B63. Dielectric properties of proton-disordered ice Ih from classical molecular dynamics simulations**

Xun Wang, Kenneth D. Jordan

**B64. Geminal-augmented multiconfigurational self-consistent field theory for n-electron systems**

Nicholas J. Ward, Andrew Komornicki, Liguo Kong, Todd J. Martínez

**B65. On-the-fly ab initio semiclassical dynamics: Emission spectra of oligothiophenes**

Marius Wehrle, Miroslav Sulc, Jiri Vanicek

**B66. Modeling defects in germanium nanowires**

Alicia Welden, Dominika Zgid

**B67. Variational quantum embedding in symmetry-restored mean fields**

Matthew Welborn, Takashi Tsuchimochi, Troy Van Voorhis

**B68. Molecular insight at heterojunction interface of polymer-fullerene organic photovoltaic (OPV) : A multi-scale atomistic simulation study**

Shuhao Wen, David Mc Mahon, Troy Van Voorhis

**B69. Dynamics simulations of gas-phase ion-molecule reactions - Investigating the micro-solvation effect**

Jing Xie, William L. Hase

**B70. What is that bond? Understanding chemical bonds with generalized valence bond theory**

Lu T. Xu, Tyler Y Takeshita, Thom H. Dunning, Jr.

**B71. Strategies to improve CZTS crystal quality for thin film solar cells: A computational study**

Kuang Yu, Emily A. Carter

**B72. Improving the accuracy and efficiency of time-resolved electronic spectra calculations: Cellular dephasing representation with a prefactor**

Eduardo Zambrano, Miroslav Sulc, Jiri Vanicek

**B73. Roles of the low-lying electronic states of pentacene in its singlet fission and seeking smaller singlet fission chromophores**

Tao Zeng, Roald Hoffmann, Nandini Ananth

**B74. Designed crystalline and disordered classical ground states of matter**

Ge Zhang, Frank H. Stillinger, Salvatore Torquato

B75. Correlating the structure and catalytic function of nanoparticles

Liang Zhang, Graeme Henkelman

**B76. Investigation on the self-cleavage reaction in *glmS* ribozyme by quantum mechanical/molecular mechanical free energy simulations**

Sixue Zhang, Sharon Hammes-Schiffer

B77. Estimating rate coefficients for fluctuating decay processes

Helen C. Zhao, Shane W. Flynn, Jason R. Green

**B78. Free-energy based Monte Carlo simulations of a model microphase former**

Yuan Zhuang, Patrick Charbonneau