MONDAY, AUGUST 29		
Poster #	**Title**	**Authors**
M1	*New developments for many-core technologies to accelerate Density Functional Theory calculations of molecular crystal polymorphs with numerical basis sets*	Álvaro Vazquez-Mayagoitia, Argonne Leadership Computing Facility
M2	*Quantum Vibration Perturbation Theory: For On-the-Fly Computation of Vibrational Frequencies of Local Modes in the Condensed Phase*	Adam Grofe, University of Minnesota Katelyn Youmans, University of Minnesota Hui Li, Jilin University Gao Jiali, University of Minnesota
M3	*Local Compressibility: Ground-State Predictions of Quantum Yield Trends in Azobenzene-Modified DNA*	Addie Kingsland, University of Washington Soumyadyuti Samai, University of Washington Yunqi Yan, University of Washington David Ginger, University of Washington Lutz Maibaum, University of Washington
M4		
M5	*Modeling Molecular Motors on Metal Surfaces*	Melihat Madran, Sabanci University Sondan Durukanoglu, Sabanci University Zehra Akdeniz, Piri Reis University Alimet Sema Ozen, Piri Reis University
M6	*Probing electronic wave functions of sodium-doped clusters: Dyson orbitals, anisotropy parameters, and ionization cross-sections*	Anastasia Gunina, Department of Chemistry, University of Southern Californnia Anna Krylov, Department of Chemistry, University of Southern Californnia
M7	*Force Field Development for Conjugated Polymers: Molecular Dynamics Validation with Neutron and X-ray Scattering*	Caitlyn Wolf, University of Washington Kiran Kanekal, University of Washington Yeneneh Yimer, University of Washington Lilo Pozzo, University of Washington
M8	*Signatures of Magnetic Plasmon Hybridization and Magnetic-Magnetic Fano Resonances in Electron Energy Loss Spectroscopy*	Charles Chergui, University of Washington David Masiello, University of Washington
M9	*Determination of Desorption and Adsorption Barriers of CO on Pt(111) in the Free Energy Landscape from First Principles Calculations: An Answer of CO Puzzle*	Chenxi Guo, Queen's University Belfast Peijun Hu, Queen's University Belfast
M10	*Scalable Dual Basis Explicitly Correlated Coupled-Cluster Methods Using the TiledArray Framework*	Chong Peng, Virginia Tech Edward Valeev, Virginia Tech
M11	*Many-Body Energies and Energy Decomposition of Non-Covalent Complexes and Clusters with Subsystem DFT*	Christian Muck-Lichtenfeld, University of Muenster Jan P. Unsleber, University of Muenster Johannes Neugebauer, University of Muenster
M12	*Structural elucidation of a novel alkaloid from \textit{Uncaria tomentosa}*	Felipe Vargas, University of Costa Rica William Zamora, University of Costa Rica Renato Murillo, University of Costa Rica Mirtha Navarro, University of Costa Rica Cristopher Camacho, University of Costa Rica
M13	*First-Principles Modeling of Coherent Exciton Transfer in Binuclear Pt(II) complexes*	David Lingerfelt, University of Washinton Patrick Lestrange, University of Washinton Xiaosong Li, University of Washinton
M14	*Efficient Implementation of the Chebyshev Propagator in Quantum Electronic Dynamics*	David Williams-Young, University of Washington Xiaosong Li, University of Washington
M15	*Optimal temperature set for Replica Exchange sampling*	Dominik Gront, Uniwersity of Warsaw, Faculty of Chemistry
M16	*Quantitative thermochemistry of metalloactinides. A coupled cluster comparison of UO3 and PtUO2*	Elise Held, Washington State University Kirk Peterson, Washington State University

M17	*Cleavage pattern of mixed linkage (1,3;1,4)-β-D-glucans by a soil metagenome derived GH16*	Erica Prates, Institute of Chemistry, UNICAMP Thabata Alvarez, Brazilian Bioethanol Science and Technology Laboratory Marcelo Liberato, Brazilian Bioethanol Science and Technology Laboratory Igor Polikarpov, Sao Carlos Institute of Physics, University of Sao Paulo Fabio Squina, Brazilian Bioethanol Science and Technology Laboratory
M18	*Methane Steam Reforming: Using External Electric Fields to Enhance the Catalytic Performance of Ni-based Catalysts*	Fanglin Che, Washington State University Jake Gray, Washington State University Su Ha, Washington State University Jean-Sabin McEwen, Washington State University
M19	*On the Electronic States of Selenium Monoiodide, SeI*	Antonio Ricardo Belinassi, Universidade de São Paulo, Instituto de Química, Departamento deQuímica Fundamental Tiago Vinicius Alves, Universidade Federal da Bahia, Instituto de Químicaa, Departamento de Físico-Química Fernando Ornellas, Universidade de São Paulo, Instituto de Química, Departamento de Química Fundamental
M20	*Analyzing the Hydration Structure of HIV-1 Protease using Molecular Dynamics Simulations*	Florian Leidner, University of Massachusetts Medical School Janet Paulsen, University of Massachusetts Medical School Celia Schiffer, University of Massachusetts Medical School
M21	*Polaron Pair Formation and Dynamics in a Oligothiophene Model Explored by Coupling Ehrenfest Dynamics and Time-Resolved Vibrational Analysis*	Greta Donati, Department of Chemistry, University of Washington Dipartimento di Scienze Chimiche, Università degli Studi di Napoli Federico II, Complesso Universitario di M.S.Angelo David B. Lingerfelt , Department of Chemistry, University of Washington Alessio Petrone, Department of Chemistry, University of Washington Nadia Rega, Dipartimento di Scienze Chimiche, Università degli Studi di Napoli Federico II, Complesso Universitario di M.S.Angelo Italian Institute of Technology, IIT@CRIB Center for Advanced Biomaterials for Healthcare, Largo Barsanti e Matteucci Xiaosong Li, Department of Chemistry, University of Washington
M22	*Local Multi-Resonance Description of Excited States in Quantum Monte Carlo*	Habiburrahman Zulfikri, University of Twente Claudia Filippi, University of Twente
M23	*Computational Studies of the Electronic Structures of Copper-Doped CdSe Nanocrystals*	Heidi Nelson, University of Washington Xiaosong Li, University of Washington Daniel Gamelin, University of Washington
M24	*Electron localization function as a physicochemical tool for predicting hydrogen absorption abilities of nano alloy materials*	Aya Matsuda, Ochanomizu University Hirotoshi Mori, Ochanomizu University
M25	*QM/MM model for the transglutaminase reaction of blood coagulation factor XIII; the first (acyl-enzyme formation) step*	Istvan Komaromi, University of Debrecen, Faculty of Medicine, Department of Laboratory Medicine, Division of Clinical Laboratory Science Gabor Balogh, University of Debrecen, Faculty of Medicine, Department of Laboratory Medicine, Division of Clinical Laboratory Science
M26	*Rotational energy transfer in collisions of ammonia with rare gas atoms and H2*	Jerome Loreau, Université Libre de Bruxelles (ULB) Ad van der Avoird, Radboud University
M27	*Benchmark study on the electronic structure properties of polyoxometalate (POM) Keggin-like structures at Carbon substrates for energy storage applications*	Jesus Muniz, Universidad Nacional Autónoma de México Christian Celaya, Universidad Nacional Autónoma de México Ana-Karina Cuentas-Gallegos, Universidad Nacional Autónoma de México Luis-Martin Mejia, Universidad Nacional Autónoma de México Miguel Robles, Universidad Nacional Autónoma de México Maximiliano Valdez, Universidad Nacional Autónoma de México

M28	*Perturbative universal state-selective correction for state-specific multi-reference coupled cluster methods*	Jiri Brabec, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic Subrata Banik, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic Karol Kowalski, William R. Wiley Environmental Molecular Sciences Laboratory, Battelle, Pacific Northwest National Laboratory Ondrej Demel, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic Jiri Pittner, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic
M29	*A Nexus between Theory and Experiment: Non-empirical Quantum Mechanical Computational Methodology Applied to Cucurbit[n]uril•Guest Binding Interactions*	Jiri Hostas, IOCB Prague David Sigwalt, University of Maryland Marina Sekutor, RuÄ‘er BoÅ¡koviÄ‡ Institute Haresh Ajani, IOCB Prague Jan Rezac, IOCB Prague Matus Dubecky, Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute Peter Y. Zavalij, University of Maryland Kata Mlinarić-Majerski, Ruđer Bošković Institute Lyle Isaacs, University of Maryland Robert Glaser, Ben-Gurion University of the Negev Pavel Hobza, IOCB Prague
M30	*Molecular dynamics with non-adiabatic and spin-orbit effects*	Marek Pederzoli, J. Heyrovsky Institute Jiri Pittner, J. Heyrovsky Institute
M31	*Time-Dependent Density Functional Theory Calculations of Electronic Circular Dichroism for Phenylalanine and Hydrated Clusters*	Jiyoung Heo, Sangmyung University Heeseon Jang, Chungbuk National University
M32	*Catalytic Activity in Ethylene Polymerization Processes understood through the Local Hyper-Softness*	Jorge Martinez-Araya, Universidad Andres Bello Andre Grand, CEA University Grenoble Alpes Daniel Glossman-Mitnik, Centro de InvestigaciÃ³n en Materiales Avanzados
M33	*Real Time Propagation of the Exact Relativistic Two Component Equations*	Joshua Goings, University of Washington Joseph Kasper, University of Washington Franco Egidi, University of Washington Xiaosong Li, University of Washington
M34	*Theoretical study of fluorinated, chlorinated, and brominated halocarbons*	Kameron Jorgensen, Texas A&M International University
M35	*The effect of water molecules on the binding affinity of the ligands to the HIV-1 antibody 2G12*	Kaori Noto, Kitasato University Keiko Takano, Ochanomizu University
M36	*The Effect of Membrane-Mediated Interactions among Membrane-Bound Proteins*	Kayla Sapp, University of Washington Lutz Maibaum, University of Washington
M37	*Hydrogen Bond Network Dynamics with Nuclear Quantum Effects*	Lance Edens, Washington State University Ondrej Marsalek, Stanford University Thomas Markland, Stanford University Christine Isborn, University of California, Merced Aurora Clark, Washington State University
M38	*Elucidating metal oxide cluster spectra through projection theories*	Lee Thompson, University of California, Merced Hrant Hratchian, University of California, Merced
M39	*Asymmetric behavior of Human Topoisomerase IIÎ² in G-segment DNA opening*	Levent Sari, School of Medicine, Fatih University, Istanbul Riza Akyuz, Department of Physics, Fatih University, Istanbul
M40	*Analytical treatments of the anharmonic effects observed in the infrared spectra of small, organic ions*	Lindsey R. Madison, University of Washington Anne B. McCoy, University of Washington

M41	*The Excitonic Signature of LH2: from a Multiscale ab initio Description to experimental evidences*	Lorenzo Cupellini, Dipartimento di Chimica e Chimica Industriale, University of Pisa Sandro Jurinovich, Dipartimento di Chimica e Chimica Industriale, University of Pisa Stefano Caprasecca, Dipartimento di Chimica e Chimica Industriale, University of Pisa Ciro Achille Guido, Dipartimento di Chimica e Chimica Industriale, University of Pisa Marco Campetella, Dipartimento di Chimica e Chimica Industriale, University of Pisa Alastair Gardiner, Institute of Molecular, Cell and Systems Biology, College of Medical Veterinary and Life Sciences, University of Glasgow Richard J Cogdell, Institute of Molecular, Cell and Systems Biology, College of Medical Veterinary and Life Sciences, University of Glasgow Benedetta Mennucci, Dipartimento di Chimica e Chimica Industriale, University of Pisa
M42	*Calculating chemical reaction rates through metadynamics simulations*	Luiz Oliveira, University of Washington Christopher Fu, University of Washington Jim Pfaendtner, University of Washington
M43	*Novel Cationic Mo-Alkylidene Catalysts Can Tolerate Functional Groups in Olefin Metathesis*	Maren Podewitz, University of Innsbruck Michael R. Buchmeiser, University of Stuttgart Klaus R. Liedl, University of Innsbruck
M44	*Time resolved vibrational analysis to reveal the origin of Pyranine photoreactivity*	Maria Gabriella Chiariello, Department of Chemical Sciences, University of Napoli 'Federico II' Greta Donati, Department of Chemical Sciences, University of Napoli 'Federico II' Nadia Rega, Department of Chemical Sciences, University of Napoli 'Federico II'; IIT@CRIB Center for Advanced Biomaterials for Healthcare
M45	*Unlocking New Potentials: Improving the Accuracy, Transferability, and Robustness of Ab Initio Intermolecular Force Fields*	Mary Van Vleet, University of Wisconsin-Madison Alston Misquitta, Queen Mary University of London Anthony Stone, University of Cambridge J.R. Schmidt, University of Wisconsin-Madison
M46	*Ground State Properties of Small and Large Charge Carrier Complexes in 2D Transition Metal Dichalcogenides via Diffusion Monte Carlo*	Matthew Mayers, Columbia University David Reichman, Columbia University
M47	*Torsion-Vibrational Couplings in Methyl Peroxy Radicals*	Meng Huang, The Ohio State University Terry Miller, The Ohio State University Anne McCoy, University of Washington
M48	*Calculations of cesium doped molybdenum materials for nuclear fusion applications*	Michal Novotny, Comenius University Ivan Cernusak
M49	*Benchmark Study of Performance of Density Functional Theory for Molecular Properties of Li2Sn (n=1~8) clusters*	Myoungju Chae, Department of Chemistry, The Catholic University of Korea Jiwon Moon, Department of Chemistry, The Catholic University of Korea Joonghan Kim, Department of Chemistry, The Catholic University of Korea
M50	*A theoretical and experimental study on structures and properties of novel transition metal complexes of which coordination numbers are controlled without steric hindrance*	Nahoko Kuroki, Ochanomizu University Koichiro Takao, Tokyo Institute of Technology Hirotoshi Mori, Ochanomizu University
M51	*Sensitivity in relative binding free energies from incremental ligand changes within a simple model binding site using modern free energy calculation protocols and force fields*	Nathan Lim, University of California, Irvine Lingle Wang, Schrodinger Robert Abel, Schrodinger David Mobley, University of California, Irvine
M52	*EELS imaging of noble-catalytic metal hybrid systems for plasmon mediated catalysis*	Nicholas Montoni, University of Washington Department of Chemistry David Masiello, University of Washington Department of Chemistry
M53	*Modelling of the electronic states of Si quantum dots through DFT & TD-DFT methods*	Nicolas Iacobellis, Université Libre de Bruxelles Nathalie Vaeck, Université Libre de Bruxelles

M54	*Geometrically Designing the Ideal Environment for Perovskite Dopants*	Nicole Onishi, Western Washington University Robert Berger, Western Washington University
M55	*Single Gold Nanorod Absorption Spectroscopy with Whispering Gallery Modes*	Niket Thakkar, University of Washington Applied Mathematics David Masiello, University of Washington Chemistry
M56	*Dimeric Conformation Sensitive Low-Lying Electronic Excited States of Tetracene Congeners and Their Significance in Singlet Fission*	Nikhil Aggarwal, Department of Chemistry, Indian Institute of Technology-Madras Archita Patnaik, Department of Chemistry, Indian Institute of Technology-Madras
M57	*Test calculations of spectroscopic signals from small molecules in cryogenic matrices*	Philip Kovac, University of Oregon Jeffrey Cina, University of Oregon
M58	*Correlation consistent basis sets for lanthanides. The atoms La – Lu*	Qing Lu, Washington State University Kirk Peterson, Washington State University
M59	*Coupled cluster investigations of the photodetachment spectra of the UO2X– and UO2X2– anions (X=F, Cl)*	Rolf Hermanson, Washington State University Kirk Peterson, Washington State University
M60	*Kinetic Evaluation of Doped Hercynite for Two Step Solar Thermochemcial Water-Splitting*	Ryan Trottier, University of Colorado Boulder Samantha Miller, University of Colorado Boulder Charles Musgrave, University of Colorado Boulder
M61	*Application of ab initio many-body perturbation theory with Gaussian basis sets to charged and neutral excitations in organic molecules*	Samia Hamed, University of California, Berkeley Tonatiuh Rangel, University of California, Berkeley Fabien Bruneval, Service de Recherches de Métallurgie Physique, CEA, DEN, Université Paris-Saclay Jeffrey Neaton, University of California, Berkeley
M62	*Development of a Polarizable Block Model Potential Function for DNA*	Setsuko Nakagawa, Kinjo Gakuin University
M63	*Theoretical Study on Relative Stability of Indigo and its Isomers*	Seung Joo Cho Chosun University, South Korea
M64	*The two-photon absorption cross-section of solution-phase p-nitroaniline: investigation of the effects of solvation models*	Shih-I Lu, Soochow University
M65	*Computational Structure Analysis and Virtual Inhibitor Design Targeting the Active Site of APOBEC3B*	Shurong Hou, University of Massachusetts Medical School Tania Silvas, University of Massachusetts Medical School Takahide Kono, University of Massachusetts Medical School Ellen Nalivaika, University of Massachusetts Medical School Nese Yilmaz, University of Massachusetts Medical School Celia Schiffer, University of Massachusetts Medical School
M66	*Single ion solvation free energies with ab initio molecular dynamics*	Timothy Duignan, Pacific Northwest National Laboratory Marcel Baer, Pacific Northwest National Laboratory Gregory Schenter, Pacific Northwest National Laboratory Christopher Mundy, Pacific Northwest National Laboratory
M67	*Atomistic Study of Curcumin Impact on Amyloid-Î²² Aggregation*	Tye Martin, University of New Mexico Angelina Malagodi, Macalester College Eva Chi, University of New Mexico Deborah Evans, University of New Mexico
M68	*Ab initio molecular dynamics to explore different time scales in a complex reaction space: the simulation of Excited State Proton Transfer in condensed phase*	Umberto Raucci, University Federico II of Napoli Nadia Rega, University Federico II of Napoli; Italian Institute of Technology, IIT@CRIB Center for Advanced Biomaterials for Healthcare
M69	*Quantum chemical characterization of small molecule activation reactions catalyzed by transition metals*	Varinia Bernales, Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota Konstantinos Vogiatzis, Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota Laura Gagliardi, Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota
M70	*Improving upon approximate CCSD methods: how to add higher excitations?*	Varun Rishi, Quantum Theory Project, University Of Florida Ajith Perera, Quantum Theory Project, University Of Florida Rodney Bartlett, Quantum Theory Project, University Of Florida
M71	*Improved Exchange Coupling Constants and Spin Crossover Gaps for Transition Metal Complexes Using Spin Projection*	Xianghai Sheng, University of California, Merced Lee Thompson, University of California, Merced Hrant Hratchian, University of California, Merced

M72	*The QTP Family of Density Functional Theory with Extended Applicability*	Yifan Jin, University of Florida Rodney Bartlett, University of Florida
M73	*Global Potential Energy Surfaces of Quintet, Triplet, and Singlet O4*	Yuliya Paukku, University of Minnesota Zoltan Varga, University of Minnesota Guoliang Song, Fudan University Ruben Meana-Paneda, University of Minnesota Bo Long, University of Minnesota Thomas Schwartzentruber, University of Minnesota Graham Candler, University of Minnesota Donald Truhlar, University of Minnesota
M74	*Unraveling the underlying absorption and emission mechanism of nitrogen doping graphene quantum dots*	Xianghong Niu, Southeast University, Nanjing Yuqing Zhou, Southeast University, Nanjing Jinlan Wang, Southeast University, Nanjing
M75	*An Introduction to the MMPT Force Field Method for Simulating Reactivity, Infrared Spectra and Grotthuss Mechanism of Reactive Systems with Excess Active Protons*	Zhen-Hap Xu, University of Basel Markus Meuwly, University of Basel
M76	*Investigating the Mechanism and Kinetics of Fischer-Tropsch Process on a Stepped Cobalt Surface using First Principles Calculation and Micro-Kinetic Simulations*	Zihao Yao, Queen's University Belfast Peijun Hu, Queen's University Belfast

TUESDAY, AUGUST 30		
Poster #	**Title**	**Authors**
T1	*Charge Separation in Donor-Acceptor Dyads: The Role of High-Energy Charge Transfer States*	Aleksey Kocherzhenko, University of California, Merced Donghyun Lee, University of California, Berkeley Michael Forsuelo, University of California, Berkeley Christine Isborn, University of California, Merced Birgitta Whaley, University of California, Berkeley
T2	*Modeling excited states of large molecular systems using hybrid QM/QM methods with point charge embedding*	Alessandro Biancardi, The University of Kansas Jeremy Barnes, The University of Kansas, Park University Marco Caricato, The University of Kansas
T3	*Solute interactions and phase partitioning at the Aqueous:Organic interface*	Alex McCue, Department of Chemistry, Washington State University Aurora Clark, Departiment of Chemistry, Washington State Unviersity
T4	*Self-hydrogenation and self-metalation of tetraphenyl porphyrin at TiO2(110)*	Mikel Abadia, CSIC-UPV/EHU, San Sebastian, Spain Maurizio Casarin, Universita di Padova, Padova, Italy Marcos Dominguez, University of Trieste, Trieste, Italy Luca Floreano, CNR-IOM, Trieste, Italy Daniel Forrer, CNR-ICMATE, Padova, Italy Giacomo Lovat, University of Trieste, Trieste, Italy Celia Rogero, CSIC-UPV/EHU, San Sebastian, Spain Andrea Vittadini, CNR-ICMATE, Padova, Italy
T5	*Modelling surface desorption processes for cometary chemistry and astrochemistry*	Andrew Gibbons, Universite Libre de Bruxelles (ULB) / Royal Belgian Institute for Space Aeronomy (BIRA-IASB) Johan De Keyser, Royal Belgian Institute for Space Aeronomy (BIRA-IASB) Gaël Cessateur, Royal Belgian Institute for Space Aeronomy (BIRA-IASB) Frederik Dhooghe, Royal Belgian Institute for Space Aeronomy (BIRA-IASB) Herbert Gunell, Royal Belgian Institute for Space Aeronomy (BIRA-IASB) Jerome Loreau, Universite Libre de Bruxelles (ULB) Romain Maggiolo, Royal Belgian Institute for Space Aeronomy (BIRA-IASB) Nathalie Vaeck, Universite Libre de Bruxelles (ULB)
T6	*Bridging Hydrogen Atom Transfer and Electron-Proton Transfer*	Aparna Karippara Harshan, University of Illinois at Urbana Champaign Alexander Soudackov, University of Illinois at Urbana Champaign Sharon Hammes-Schiffer, University of Illinois at Urbana Champaign
T7	*Construction of dynamic coarse-grained models with realistic short time behavior that accurately describe translational and rotational diffusion*	Aram Davtyan, Department of Chemistry, The James Franck Institute, Institute for Biophysical Dynamics and Computation Institute, The University of Chicago Gregory Voth, Department of Chemistry, The James Franck Institute, Institute for Biophysical Dynamics and Computation Institute, The University of Chicago Hans Andersen , Department of Chemistry, Stanford University
T8	*Determining Energy Barriers and Pathway Selectivities from Metadynamics*	Christopher Fu, University of Washington Jim Pfaendtner, University of Washington
T9	*DFT Approach for Understanding of Magnetic Interactions in Organic High-spin Molecules*	Daeheum Cho, Sungkyunkwan University Kyoung Chul Ko, Sungkyunkwan University Yeonsig Nam, Sungkyunkwan University Jin Yong Lee, Sungkyunkwan University
T10	*A model for ultra-fast charge transport in membrane proteins*	Sheh-Yi Sheu, Department of Life Sciences and Institute of Genome Sciences, National Yang-Ming University Dah-Yen Yang, Institute of Atomic and Molecular Sciences, Academia Sinica
T11	*Quantifying Energetic Reaction Barriers with Quantum Monte Carlo*	Ellen Swann, CSIRO, Australia Manolo Per, CSIRO, Australia Amanda Barnard, CSIRO, Australia Michelle Coote, Australian National University
T12	*Odd order dispersion interactions in the effective fragment potential method*	Emilie Guidez, Iowa State University Mark Gordon, Iowa State University

T13	*Electron-Nuclear Dynamics: New implementations with Plane Waves Base Functions*	Erico Souza Teixeira, Texas Tech University Jorge Morales, Texas Tech University
T14	*Accurate free energies of solvation for predicting the distribution of solutes across liquid:liquid phase boundaries*	Ernesto Martinez-Baez, Washington State University Aurora E. Clark, Washington State University
T15	*Linear scaling explicitly correlated coupled cluster methods for large molecular systems*	Fabijan Pavosevic, Virginia Tech Christoph Riplinger, Max Planck Institute for Chemical Energy Conversion Chong Peng, Virginia Tech Frank Neese, Max Planck Institute for Chemical Energy Conversion Edward F. Valeev, Virginia Tech
T16	*Partial Infinite Swapping: Implementation and Application to peptides and proteins in the Gas Phase and in Solution*	Florent Hedin, University of Basel Nuria Plattner, Free university of Berlin Jimmie D. Doll, Brown University Markus Meuwly, University of Basel
T17	*Thermal energy storage in nanofluids: what can simulations teach us?*	Francesca Costanzo, Catalan Institute of Nanoscience and Nanotechnology - ICN2, CSIC and BIST, Campus de Bellaterra Bernd Ensing, Universita of Amsterdam Pablo Ordejon, Catalan Institute of Nanoscience and Nanotechnology - ICN2, CSIC and BIST, Campus de Bellaterra
T18	*V2O5 polymorphs as multi-valent intercalation cathode materials: a first-principles study*	Gopalakrishnan Sai Gautam, Massachusetts Institute of Technology; Lawrence Berkeley National Laboratory Pieremanuele Canepa, Lawrence Berkeley National Laboratory Gerbrand Ceder, University of California Berkeley ; Lawrence Berkeley National Laboratory
T19	*Towards an efficient mean-field wave-function based theory for periodic systems*	Hai-Anh Le, Northwestern University Toru Shiozaki, Northwestern University
T20	*Potential Energy Surface Intersections for the Si(1D)H2 Reactive System: A Five-State Study*	Yanan Wu, Institute of Chemistry, Chinese Academy of Sciences Haitao Ma, Institute of Chemistry, Chinese Academy of Sciences Wensheng Bian, Institute of Chemistry, Chinese Academy of Sciences
T21	*Kinetics and Mechanism of Schiff Base Hydrolysis for the Fluorescent Detection of Water in Organic Solvents*	Hu Shi, Sungkyunkwan University Daeheum Cho, Sungkyunkwan University Jong Seung Kim, Korea University Jin Yong Lee, Sungkyunkwan University
T22	*Enhancing the kinetic stability of orthogonal bipolar hosts in organic light-emitting diodes through spiro-conjugation*	Hyeonho Choi, Samsung Advanced Institute of Technology Won-joon Son, Samsung Advanced Institute of Technology Myung-Hwan Whangbo, Department of Chemistry, North Carolina State University
T23	*Configuration interaction singles and doubles using Kohn-Sham orbitals with local exchange potential Jaechang*	Jaechang Lim, Department of Chemistry, KAIST Sunghwan Choi, Department of Chemistry, KAIST Jaewook Kim, Department of Chemistry, KAIST Woo Youn Kim, Department of Chemistry, KAIST
T24	*Role of local exact exchange potential in hybrid functionals for accurate excited state calculations*	Jaewook Kim, Department of Chemistry, KAIST Kwangwoo Hong, Department of Chemistry, KAIST Sang-Yeon Hwang, Department of Chemistry, KAIST Seongok Ryu, Department of Chemistry, KAIST Sunghwan Choi, Department of Chemistry, KAIST Woo Youn Kim, Department of Chemistry, KAIST
T25	*Interaction and Reaction of Water with 3D Neutral and Ionic Aluminum Clusters in the Gas Phase*	Jerzy Moc, Wroclaw University
T26	*Inner space perturbation theory in matrix product states: Replacing expensive iterative diagonalization*	Jiajun Ren, MOE Key Laboratory of Organic OptoElectronics and Molecular Engineering, Department of Chemistry, Tsinghua University Beijing Yuanping Yi, Key Laboratory of Organic Solids, Beijing National Laboratory for Molecular Science (BNLMS), Institute of Chemistry, Chinese Academy of Sciences Beijing Zhigang Shuai, MOE Key Laboratory of Organic OptoElectronics and Molecular Engineering, Department of Chemistry, Tsinghua University Beijing

T28	*Theoretical Investigation for the Reaction Pathway from Acetylene to Naphthalene with La Atom via La-Activated Bicyclo-Oligomerization.*	Jiwon Moon, The Catholic University of Korea, The Department of Chemistry Joonghan Kim, The Catholic University of Korea, The Department of Chemistry
T29	*Revealing the unusual reactivity of organic molecules on Si(001) surfaces leading towards internal interfaces*	Josua Pecher, Philipps-University Marburg Ralf Tonner, Philipps-University Marburg
T30	*Application of Ab Initio Multiple Spawning to transition-metal photochemistry*	Julia Preiss, Institute for Physical Chemistry, Friedrich-Schiller-University Jena Basile Curchod, Centre for Computational Chemistry, School of Chemistry, University of Bristol Todd Martinez, Department of Chemistry and PULSE Institute, Stanford University Martin Presselt, Institute for Physical Chemistry, Friedrich-Schiller-University Jena
T31	*Excited-state deactivation mechanism in Nickel-Tetra-Mesityl-Porphyrin*	Julia Preiss, Institute for Physical Chemistry, Friedrich-Schiller-University Jena Benjamin Dietzek, Institute for Physical Chemistry, Friedrich-Schiller-University Jena Todd Martinez, Department of Chemistry and PULSE Institute, Stanford University Martin Presselt, Institute for Physical Chemistry, Friedrich-Schiller-University Jena
T32	*Electron Nuclear Dynamics Elucidation of Water Radiolysis and DNA/RNA Damage Reactions in Proton Cancer Therapy*	Karthik Uppulury, Texas Tech University Austin Privett, Lipscomb University Erico Teixeira, Texas Tech University Ryan Merritt, Texas Tech University Jorge Morales, Texas Tech University
T33	*Photophysics and 1O2 Sensitization Characteristics of BODIPY Dyes for Photodynamic Therapy*	Keenan Komoto, Department of Chemistry, Western Washington University Tim Kowalczyk, Department of Chemistry, Western Washington University
T34	*Network Analysis of Nuclear Quantum Effects Upon Hydrogen Bonds in Aqueous Systems*	Lance Edens, Washington State University Lelee Ounkham, Washington State University Ondrej Marsalek, Stanford University Thomas Markland, Stanford University Christine Isborn, University of California, Merced Aurora Clark, Washington State University
T35	*Modeling Electron Anions in Glasses*	Lewis E. Johnson, Peter V. Sushko Physical and Computational Sciences Division, Pacific Northwest National Laboratory, 902 Battelle Boulevard, Richland WA 99354, USA Yudai Tomota, Hideo Hosono Materials Research Center of Element Strategy, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8053, Japan
T36	*Optimal laser impulsion for controlling vibrational and rotational population within the Ns = 1, Nr = 5 polyad of* $^{12}C_2H_2$	Ludovic Santos, Universite Libre de Bruxelles Nicolas Iacobellis, Universite Libre de Bruxelles Michel Herman, Universite Libre de Bruxelles David S. Perry, University of Akron Michèle Desouter-Lecomte, University Paris-Saclay Nathalie Vaeck, Universite Libre de Bruxelles
T37	*Evaluation of the Factors Impacting the Accuracy of 13C NMR Chemical Shifts Predictions using Density Functional Theory and its Application to Natural Product Identification*	Mark Iron, Weizmann Institute of Science

T38	*Two-dimensional photon echoes reveal the vibrational origin of vision*	Marwa H. Farag, Zernike Institute for Advanced Materials, University of Groningen Philip J. M. Johnson, Departments of Chemistry and Physics, University of Toronto Alexei Halpin, Departments of Chemistry and Physics, University of Toronto Valentyn I. Prokhorenko, Max-Planck Institute for the structure and Dynamics of Matters, Atomically Resolved Dynamics Division Jasper Knoester, Zernike Institute for Advanced Materials, University of Groningen Thomas L. C. Jansen, Zernike Institute for Advanced Materials, University of Groningen R. J. Dwayne Miller, Max-Planck Institute for the Structure and Dynamics of Matters, Atomically Resolved Dynamics Division
T39	*The Oxidative Coupling of Methane: First-principles Microkinetic Modeling*	Matthias Baldofski, Humboldt Universitaet zu Berlin Joachim Sauer, Humboldt Universitaet zu Berlin
T40	*Tunable electronic and radical nature of oligoacenes upon chemical doping: a multireference study*	Max Pinheiro Jr, Departamento de Química, Instituto Tecnologico de Aeronautica Francisco Machado, Departamento de Química, Instituto Tecnologico de Aeronautica Hans Lischka, Department of Chemistry and Biochemistry, Texas Tech University
T41	*Modeling of bio-inorganic interfaces with ab initio force fields*	Michal Trachta, Institute of Organic Chemistry and Biochemistry, AS CR Miroslav RubeÅ¡, Institute of Organic Chemistry and Biochemistry, AS CR Ota BludskÃ½, Institute of Organic Chemistry and Biochemistry, AS CR
T42	*Massively Parallel Self-Consistent Field Methods for Quantum Chemistry*	Murat Keceli, Argonne National Laboratory Hong Zhang, Argonne National Laboratory Peter Zapol, Argonne National Laboratory David Dixon, The University of Alabama Alvaro Vazquez-Mayagoitiae, Argonne National Laboratory Albert Wagner, Argonne National Laboratory
T43	*The Effect of Confinement on Solvent Structure and Dynamics in MOFs and Zeolites*	Mustafa Kucukkal, Washington State University Tiecheng Zhou, Washington State University Aurora Clark, Washington State University
T44	*Combination of multiple spectroscopy techniques using data fusion for enhanced prediction modelling of physical-mechanical properties of paper*	Najmeh Tavassoli, PhD Candidate, University of British Columbia Edward Grant, Professor, University of British Columbia Alison Bain, MSc Student, University of British Columbia Ashton Christy, MSc Student, University of British Columbia
T45	*Computational approach for studying the participation of ketodiperoxy acids in atmospheric new-particle formation*	Nanna Myllys, University of Helsinki Jonas Elm, University of Helsinki Theo KurtÃ©n, University of Helsinki Hanna VehkamÃ¤ki, University of Helsinki
T46	*Molecular Magnets: Using Spin-Flip Methods to Describe Electronic Structure and Magnetic Properties of Binuclear Copper Compounds*	Natalie Orms, University of Southern California Anna I. Krylov, University of Southern California
T47	*Crystal structure predictions from first principles*	Rafal Podeszwa, University of Silesia Wojciech Jankiewicz, University of Silesia Michael Metz, University of Delaware Krzysztof Szalewicz, University of Delaware
T48	*Theoretical Studies of the Catalytic Hydrolysis of Sarin and Nerve Agent Simulants by Cs8Nb6O19*	Robert Chapleski, Department of Chemistry, Virginia Tech Diego Troya, Department of Chemistry, Virginia Tech
T49	*Novel actinyl cation-cation interactions in the gas phase: an accurate coupled cluster study with new correlation consistent basis sets*	Rulin Feng, Washington State University Kirk Peterson, Washington State University
T50	*Accurate bond energies of actinide carbonyls. The Th(CO)n and Th(CO)n+ molecules, n=1-4*	Samuel Battey, Washington State University Kirk Peterson, Washington State University

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Poster #	**Title**	**Authors**
W1	*Theoretical (DFT) and Docking computer simulation of the complex between Divanillin and Bovine Serum Albumin (BSA).*	Aguinaldo Robinson de Souza, Sao Paulo State University Diego Venturini, Sao Paulo State University Valdecir Farias Ximenes, Sao Paulo State University Ignez Caracelli, Federal University of Sao Carlos Nelson Henrique Morgon, University of Campinas
W2	*Non-covalent interactions in large systems based on a transferable, atom-centered basis-set incompleteness correction*	Alberto Otero de la Roza, University of British Columbia Gino DiLabio, University of British Columbia
W3	*Theoretical study of the ground and excited state tautomersim in curcumin using DFT based methods*	Baljinder Grewal, CSIR-National Chemical Laboratory Debashree Ghosh, CSIR-National Chemical Laboratory
W4	*Tuning the protein-induced absorption shifts of retinal in engineered rhodopsin mimics*	Carl-Mikael Suomivuori, University of Helsinki Lucas Lang, Technische Universität München Ana P. Gamiz-Hernandez, Technische Universität München Dage Sundholm, University of Helsinki Ville R. I. Kaila, Technische Universität München
W5	*Realistic description of exciton-phonon interactions of bacteriochlorophyll a in Fenna-Matthews-Olson complex*	Chang Woo Kim, Center for Self-Assembly and Complexity, Institute for Basic Science (IBS); Department of Chemistry, Pohang University of Science and Technology (POSTECH) Young Min Rhee, Center for Self-Assembly and Complexity, Institute for Basic Science (IBS); Department of Chemistry, Pohang University of Science and Technology (POSTECH)
W6	*Bio-inspired Design and Computational Prediction of Iron Complexes with Pendant Amines for the Production of Methanol from CO2 and H2*	Xiangyang Chen, Institute of Chemistry, Chinese Academy of Sciences Xinzheng Yang, Institute of Chemistry, Chinese Academy of Sciences
W7	*Cubic Scaling SOS-MP2 Energy and Analytic Gradients with Atomic Orbital Based Tensor Hyper-Contraction*	Chenchen Song, Stanford University Todd Martinez, Stanford University
W8	*Hydrogen Bonding in Hydrolysis Reactions*	Chin-Hui Yu, National Tsing Hua University Timm Lankau, National Tsing Hua University
W9	*Novel And Effecient Photoswitches Based On Multiazobenzenes*	Chong Yang, Heildeberg University Andreas Dreuw, Heildeberg University
W10	*Theoretical studies on the metal-metal multiple bonding in actinide dimetallocenes*	Cong-Zhi Wang, Institute of High Energy Physics, Chinese Academy of Sciences John K. Gibson, Chemical Sciences Division, Lawrence Berkeley National Laboratory Jian-Hui Lan, Institute of High Energy Physics, Chinese Academy of Sciences Qun-Yan Wu, Institute of High Energy Physics, Chinese Academy of Sciences Zhi-Fang Chai, Institute of High Energy Physics, Chinese Academy of Sciences Wei-Qun Shi, Institute of High Energy Physics, Chinese Academy of Sciences
W11	*Linear absorption spectra from explicitly time-dependent second-order approximate coupled-cluster theory*	Daniel Nascimento, Florida State University A. Eugene DePrince, III, Florida State University
W12	*On the intrinsic flexibility of the μ opioid receptor through multiscale modeling approaches*	Mathieu Fossepre, University of Namur Laurence Leherte, University of Namur Aatto Laaksonen, Stockholm University Daniel Vercauteren, University of Namur
W13	*Electronic Absorption Spectra from ab initio QM/MM and QM Molecular Dynamics: Solvent Effects on the Spectra of Coumarin and Coumarin Derivatives*	David Sanchez, Stanford University Todd Martinez, Stanford University
W14	*Adventures in the Vacuum Ultraviolet*	David Schwenke, NASA Ames Research Center

W15	*Methanol Activation Catalyzed by Small Earth-Alkali Mixed Silicon Clusters Sim-nMn with M = Be, Mg, Ca and m = 3 – 4, n = 0 – 1*	Dieu Hang Tran, Ku Leuven Minh Tho Nguyen, Ku Leuven
W16	*Local correlation studies of Br2(H2O)n=4,5 clusters and Br2@51262, Br2@51263 clathrate cages.*	Fidel Alejandro Batista Romero, Universidad Autónoma del Estado de Morelos, Mexico Antonio Gamboa Suárez, Universidad Autónoma del Estado de Morelos, Mexico Pedro Pajon-Suarez, InSTEC, Cuba Margarita Isabel Bernal Uruchurtu, Universidad Autónoma del Estado de Morelos, Mexico Ramon Hernández Lamoneda, Universidad Autónoma del Estado de Morelos, Mexico
W17	*Theoretical studies of nanoparticles with flexible structures*	Guangfeng Wei, Tongji University Zhipan Liu, Fudan University
W18	*Structure and Dynamics of the Hematite(001)-Liquid Water Interface: Hydrogen Bond Patterns, Termination Acidity and Proton Transfer*	Guido Falk von Rudorff, University College London Rasmus Jakobsen, University College London Kevin M Rosso, Pacific Northwest National Laboratory Jochen Blumberger, University College London
W19	*Accelerating hybrid density functional-based molecular dynamics simulation*	Guido Falk von Rudorff, University College London Rasmus Jakobsen, University College London Kevin M Rosso, Pacific Northwest National Laboratory Jochen Blumberger, University College London
W20	*Interaction of the first trans-membrane segment of NS2 protein with a POPC lipid bilayer*	Hung Minh Huynh, KU Leuven Minh Nguyen, KU Leuven
W21	*Automatic Fragmentation Schemes for SCF Guess Density Matrices*	Jason Ford, Stanford University Todd Martinez, Stanford University
W22	*Randomized Factorization of High-Order ERI Tensors*	Jimmy Yu, Biophysics Program, Stanford University Robert Parrish, Department of Chemistry and the PULSE Institute, Stanford University Todd Martinez, Department of Chemistry and the PULSE Institute, Stanford University
W23	*New and Highly Active Catalyst Based on Two-dimensional Nanosheets for Hydrogen Evolution Reaction*	Jinlan Wang, Southeast University
W24	*Effective vibronic models adapted to flexible medium-large chromophores*	Julien Bloino, CNR-ICCOM Alberto Baiardi, Scuola Normale Superiore
W25	*Chemical Activation Theory Employing System-Specific Quantum RRK Theory Calibrated by Variational Transition State Theory: Kinetics of Hydrogen Radical Reactions with Toluene*	Junwei Bao, University of Minnesota, Twin cities Jingjing Zheng, Gaussian, Inc. Donald Truhlar, University of Minnesota, Twin cities
W26	*Discovering Mechanisms for Perfume Discoloration using ab initio Molecular Dynamics Simulations*	Laszlo Seress, Stanford University Todd Martinez, Stanford University
W27	*Charge Transport Properties in Mixed-Stack Crystals: Super-exchange Coupling and Non-local Electron-Phonon Couplings Beyond Gamma-point*	Lingyun Zhu, National Center for Nanoscience and Technology Hua Geng, Institute of Chemistry, Chinese Academy of Sciences Yuanping Yi, Institute of Chemistry, Chinese Academy of Sciences Zhixiang Wei, National Center for Nanoscience and Technology
W28	*Shear-Slip Transitions in Polytypes: Aspirin as a Case Study*	Luc LeBlanc, Department of Chemistry, Dalhousie University Alberto Otero-de-la-Roza, National Institute for Nanotechnology, National Research Council of Canada Erin Johnson, Department of Chemistry, Dalhousie University
W29	*Evaluation of Electronic Coupling in Solids with DFT and PBC Calculations*	Alessandro Biancardi, University of Kansas Marco Caricato, University of Kansas
W30		
W31	*Graphene-Metal Interactions Using the Exchange-Hole Dipole Moment Model of Dispersion*	Matthew Christian, Dalhousie University Erin Johnson, Dalhousie University
W32	*Amyloid-β fibrils remodeling by an organic molecule: Insight from all-atomic Molecular Dynamics Simulations*	Nikhil Agrawal, University of Kwazulu-natal Adam Skelton, University of Kwazulu-natal

W33	*Fully Numerical Grid-Based Fast Multipole Method SCF Implementation*	Pauli Parkkinen, University of Helsinki Eelis Solala, University of Helsinki Wen-Hua Xu, University of Helsinki Sergio Losilla, University of Helsinki Elias Toivanen, University of Helsinki Dage Sundholm, University of Helsinki
W34	*From intermolecular interaction to intramolecular interaction, the energy decomposition analysis scheme GKS-EDA and the further development*	Peifeng Su, Xiamen University
W35	*Mechanism of Methylation of 8-Oxoguanine and Its Biological Implications: A Quantum Computational Study*	Pradeep Kumar Shukla, Assam University
W36	*Theoretical Prediction of Reverse Intersystem Crossing Rates in Organic Emitters Exploiting Thermally Activated Delayed Fluorescence*	Pralok Kumar Samanta, King Abdullah University of Science and Technology Veaceslav Coropceanu, Georgia Institute of Technology Jean-Luc Bredas, King Abdullah University of Science and Technology
W37	*Hydrogen Adsorption, Dissociation, and Spillover on Co Sub-nanoparticles Supported on t-ZrO2(101) Surface*	Qilong Xie, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Qiang Wang, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Zhonyi Ma, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Hou Bo, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Deabo Li, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry
W38	*Mechanistic Insight into the C2 Hydrocarbons Formation from Syngas on Co(111) Surface*	Qiang Wang, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Congbiao Chen, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry LItao Jia, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Hou Bo, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Debao Li, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry
W39	*Hydrogen Adsorption, Dissociation, and Spillover on Co Sub-nanoparticles Supported on t-ZrO2(101) Surface*	Qilong Xie, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Qiang wang, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Zhongyi Ma, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Bo Hou, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry Debao Li, State Key Laboratory of Coal Conversion, Institute of Coal Chemistry
W40	*Theoretical Insights into the Nature of the Bonding and Stabilities of a Series of Low-oxidation Actinide Complexes*	Qun-Yan Wu, Institute of High Energy Physics, CAS Cong-Zhi Wang, Institute of High Energy Physics, CAS Jian-Hui Lan, Institute of High Energy Physics, CAS Zhi-Fang Chai, Institute of High Energy Physics, CAS Wei-Qun Shi, Institute of High Energy Physics, CAS
W41	*Incremental Techniques for the Acceleration of SCF and TD-DFT Methods*	Robert Parrish, Stanford University Todd Martinez, Stanford University
W42	*Quantum Chemical Modeling of Water Oxidation Catalysis*	Rong-Zhen Liao, Huazhong University of Science and Technology

W43	*Ganglioside and protein-ganglioside interactions in Martini and atomistic molecular dynamics simulations*	Ruo-Xu Gu, Centre for Molecular Simulation and Department of Biological Sciences, University of Calgary Helgi IngÃ³lfsson, Groningen Biomolecular Sciences and Biotechnology (GBB) & Institute and Zernike Institute for Advanced Materials, University of Groningen Alex de Vries, Groningen Biomolecular Sciences and Biotechnology (GBB) & Institute and Zernike Institute for Advanced Materials, University of Groningen Siewert-Jan Marrink, Groningen Biomolecular Sciences and Biotechnology (GBB) & Institute and Zernike Institute for Advanced Materials, University of Groningen D. Peter Tieleman, Centre for Molecular Simulation and Department of Biological Sciences, University of Calgary
W44	*Electron-electron repulsion energy participation in non-relativistic electronic Schrödinger equation via the coupling strength parameter in Hartree-Fock theory: Analyzing the totally non-interacting reference system (TNRS)*	Sandor Kristyan, Hung. Acad. Sci. (HAS), Research Centre for Natural Sciences (RCNS)
W45	*Reduction mechanism of iron titanium based oxygen carriers with Syngas for chemical looping applications- A combined experimental and theoretical study*	Santhanamoorthi Nachimuthi, National Taiwan University of Science & Technology Yu-Cheng Liu, National Taiwan University of Science & Technology Young Ku, National Taiwan University of Science & Technology Jyh-Chiang Jiang, National Taiwan University of Science & Technology
W46	*The two faces of peptide self-assembly*	Jeseong Yoon, Seoul National University MinJun Lee, Seoul National University Young-Beom Jo, Seoul National University Youngjae Yu, Seoul National University Seokmin Shin, Seoul National University
W47	*Toward more accurate description of electrostatics in interpolation mechanics molecular mechanics: interpolation of diabatic atomic partial charges*	Seung Soo Kim, Center for Self-assembly and Complexity, Institute for Basic Science (IBS); Department of Chemistry, Pohang University of Science and Technology (POSTECH) Young Min Rhee, Center for Self-assembly and Complexity, Institute for Basic Science (IBS); Department of Chemistry, Pohang University of Science and Technology (POSTECH)
W48	*Theoretical Characterization of the Optical Properties of Organometallic Pi-Conjugated Donor-Acceptor Chromophores*	Seyhan Salman, Istanbul Bilgi University Jean-Luc Bredas, KAUST Seth Marder, Georgia Institute of Technology Veaceslav Coropceanu, Georgia Institute of Technology Stephen Barlow, Georgia Institute of Technology
W49	*All-atom semiclassical dynamics with multiple time stepping and symmetrical windowing*	Seyoung Chung, Center for Self-Assembly and Complexity, Institute for Basic Science (IBS); Department of Chemistry, Pohang University of Science and Technology (POSTECH) Young Min Rhee, Center for Self-Assembly and Complexity, Institute for Basic Science (IBS); Department of Chemistry, Pohang University of Science and Technology (POSTECH)
W50	*Developing Design Criteria for Electro-Optic Materials by Modeling* *Order in Condensed Matter*	Andreas Tillack, University of Washington, Seattle
W51	*Constructing an Intuitive Virtual Reality Interface for Ab Initio Interactive Molecular Dynamics*	Stefan Seritan, Stanford University Todd Martinez, Stanford University
W52	*That organic extra something: in silico studies on two organic-polyoxometalate hybrids*	Stefano Artin Serapian, Catalan Institute of Chemical Research, The Barcelona Institute of Science and Technology Carles Bo, Catalan Institute of Chemical Research, The Barcelona Institute of Science and Technology Guillaume Izzet, Sorbonne University, Universite Pierre et Marie Curie Anna Proust, Sorbonne University, Universite Pierre et Marie Curie

W53	*Explaining the contradictory behaviour of the solvated electron*	Stephen Dale, The University of California, Merced Erin Johnson, Dalhousie University
W54	*Thermodynamic approach to accurately determine pressure profiles for MOFs to assess their flexibility and loss of crystallinity*	Sven Rogge, Center for Molecular Modeling, Ghent University Jelle Wieme, Center for Molecular Modeling, Ghent University Louis Vanduyfhuys, Center for Molecular Modeling, Ghent University An Ghysels, Center for Molecular Modeling, Ghent University Michel Waroquier, Center for Molecular Modeling, Ghent University Toon Verstraelen, Center for Molecular Modeling, Ghent University Guillaume Maurin, Institut Charles Gerhardt Montpellier, University Montpellier Veronique Van Speybroeck, Center for Molecular Modeling, Ghent University
W55	*Modeling the Structure and Reactivity of Al(III)/Fe(III) Substitution in Kaolinite*	Tacey Hicks, Department of Chemistry and Biochemistry, Montana State University Robert Szilagyi, Department of Chemistry and Biochemistry, Montana State University
W56	*Acidity constant (pKa) calculations based on advanced MD simulations*	Thierry De Meyer, CMM - Ghent University Sven Rogge, CMM - Ghent University Bernd Ensing, HIMS - University of Amsterdam Karen De Clerck, Dept. of Textiles - Ghent University Evert Jan Meijer, HIMS - University of Amsterdam Veronique Van Speybroeck, CMM - Ghent University
W57	*Quantum dynamics calculations of systems of rotors using adiabatic approximations*	Thomas Halverson, University of Waterloo Pierre-Nicholas Roy, University of Waterloo
W58	*Vibronic Couplings for Singlet Fission in Oligoacene Dimers: A DFT Study Based on the Displaced Harmonic Oscillator Model*	Wei-Chih Chen, National Taiwan University Yuan-Chung Cheng, National Taiwan University
W59	*Identification of Reaction Coordinates and Reaction Mechanism Using the Transition Path Ensemble: From an Energy Flow Viewpoint*	Wenjin Li, The University of Illinois at Chicago Ao Ma, The University of Illinois at Chicago
W60	*Quantum chemical and kinetic modeling study for methyl-vinyl + O2 reaction*	Xi Chen, Brown University Franklin Goldsmith, Brown University
W61	*Theoretical Study of the Promiscuous Hydration and Carboxylation Activities of Phenolic Acid Decarboxylase*	Xiang Sheng, Department of Organic Chemistry, Stockholm University Fahmi Himo, Department of Organic Chemistry, Stockholm University
W62	*Automated Discovery of Complex Reaction Networks with Ab Initio Nanoreactors*	Xiaolei Zhu, Stanford University Todd Martinez, Stanford University
W63	*Nitrogen nitrogen double bond of Pyridazine cycle can Stabilize Pyridine Î±ä¸€chloro Bond*	Xiaoping Wang, Beijing Inno-Tech Medicinal Chemistry Technology Co. Ltd. Xiao Gang Song, Beijing Inno-Tech Medicinal Chemistry Technology Co. Ltd.
W64	*An Ab Initio Exciton Model Including Charge Transfer Excited States*	Xin Li, Stanford University Robert Parrish, Stanford University Fang Liu, Stanford University Sara Kokkila Schumacher, Stanford University Todd Martinez, Stanford University
W65	*Mechanistic study and computational design of non-noble metal catalysts for hydrogenation of carbon dioxide*	Xiangyang Chen, Institute of Chemistry, Chinese Academy of Sciences Xinzheng Yang, Institute of Chemistry, Chinese Academy of Sciences
W67	*Size and site dependence of the catalytic ability of thermally stable iridium subnanometer-sized clusters towards the dehydrogenation of ethane*	Yingbin Ge, Central Washington University Russell Kato, Central Washington University Prasuna Gummagatta, Central Washington University Hao Jiang, Central Washington University
W68	*Using a Spreadsheet to Solve the Schrödinger Equations for the Energies of the Ground Electronic State and the Two Lowest Excited States of H2*	Yingbin Ge, Central Washington University Robert Rittenhouse, Central Washington University Jacob Buchanan, Oregon State University Benjamin Livingston, Oregon State University

W69	*Monitoring Ultrafast Electronic Dynamics through New X-ray Spectroscopic Windows Revealed by Time-dependent Density Functional Theory Simulation*	Yu Zhang, University of California, Irvine Niranjan Govind, Pacific Northwest National Laboratory Munira Khalil, University of Washington Shaul Mukamel, University of California, Irvine
W70	*Molecular Packing and Electronic Processes for Small-Molecule Organic Solar Cells*	Yuanping Yi, Institute of Chemistry, Chinese Academy of Sciences Guangchao Han, Institute of Chemistry, Chinese Academy of Sciences Xingxing Shen, Institute of Chemistry, Chinese Academy of Sciences Yuan Guo, Institute of Chemistry, Chinese Academy of Sciences
W71	*Seniority Number in Valence Bond Theory*	Zhenhua Chen, College of Chemistry and Chemical Engineering, Xiamen University Wei Wu, College of Chemistry and Chemical Engineering, Xiamen University Chen Zhou, College of Chemistry and Chemical Engineering, Xiamen University
W72	*Nonlinear Optical Properties Described Using Damped Response Theory*	Zhongwei Hu, Pennsylvania State University Lasse Jensen, Pennsylvania State University
W73	*Modeling Circular Dichroism Spectra for Huperzine Variants: Rapid and Nondestructive Analysis Guided by TDDFT Computations*	Zikri Altun, Marmara University Donald D. Shillady, Virginia Commonwealth University Erdi A. Bleda, Marmara University Carl Trindle, University of Virginia
W74	*Multiscale Simulation of Thin-Film Lubrication*	Zuo-Bing Wu, Chinese Academy of Sciences
W75	*Computational Insights into the Reaction Mechanisms of the Synthesis of B-O Functionalized BODIPYs via Different Experimental Methods*	Petia Bobadova-Parvanova, Rockhurst University M. Graca H. Vicente, Louisiana State University Alex L. Nguyen, Louisiana State University

T51	*Ratio Based Generalised Spin Component Scaled MP2 without Counterpoise Correction Required*	Samuel Tan, Monash University Dennis Tran, Monash University Santiago Barrera Acevedo, Monash University Ekaterina Izgorodina, Monash University
T52	*Resummation of the Brillouin-Wigner Perturbation Series*	Sangyoub Lee, Seoul National University Seunghoon Lee, Seoul National University Cheol Ho Choi, Kyungpook National University
T53	*Corelike molecular properties from pseudo orbitals*	Sebastian Marquardt, Philipps-University Marburg Robert Berger, Philipps-University Marburg
T54	*The molecular mechanism of ligand unbinding from the human telomeric G-quadruplex*	Jia-Kai Zhou, Department of Life Sciences and Institute of Genome Sciences, National Yang-Ming University Dah-Yen Yang, Institute of Atomic and Molecular Sciences, Academia Sinica Sheh-Yi Sheu, Department of Life Sciences and Institute of Genome Sciences, National Yang-Ming University
T55	*The roles of auxiliary electron donors and acceptors on triphenylamine dyes for dye-sensitized solar cells: a density functional study*	Siriluk Kanchanakungwankul, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of science, Mahidol University Panida Surawatanawong, Department of Chemistry and Center of Excellence for Innovation in Chemistry, and Center of Sustainable Energy and Green Material, faculty of Science, Mahidol University
T56	*Thermodynamic Descriptors for Electrocatalytic CO2 Reduction with Transition Metal Hydrides*	Srinivasan Ramakrishnan, Stanford University Robert Waymouth, Stanford University Todd Martinez, Stanford University Christopher Chidsey, Stanford University
T57	*Taking control of the basis set error in molecular property calculations using multiwavelets*	Stig Rune Jensen, UiT - The Arctic University of Norway Luca Frediani, UiT - The Arctic University of Norway
T58	*Mechanism of CO2 absorption in amine solvents and enhancement of CO2 capture capability in blended amine solvents*	Sunkyung Kim, Sungkyunkwan University Hu Shi, Sungkyunkwan University Jin Yong Lee, Sungkyunkwan University
T59	*Ketyl Radical Formation Via Electron Proton Transfer in Aqueous Solution Versus Hydrogen Atom Transfer in Isopropanol After Photoexcitation of Aromatic Carbonyl Compounds*	Xiting Zhang, The University of Hong Kong Jiani Ma, Northwest University Songbo Li, The University of Hong Kong David Lee Phillips, The University of Hong Kong
T60	*Efficiently sampling conformations and pathways using the concurrent adaptive sampling algorithm*	Surl-Hee Ahn, Stanford University Eric Darve, Stanford University
T61	*Magnetic Couplings And Relativistic Effects In The Chemical Shift Of Paramagnetic Molecules: A First-Principles Study*	Syed Awais Rouf, NMR Research Unit, University of Oulu Jiri Mares, NMR Research Unit, University of Oulu Juha Vaara, NMR Research Unit, University of Oulu
T62	*Theoretical and Experimental Studies of Mutual Neutralization of Li+ + D-*	Thibaut Launoy, Universite Libre de Bruxelles / Universite Catholique de Louvain Arnaud Dochain, Universite Catholique de Louvain Jacques LiÃ©vin, Universite Libre de Bruxelles Jerome Loreau, Universite Libre de Bruxelles Xavier Urbain, Universite Catholique de Louvain Nathalie Vaeck, Universite Libre de Bruxelles
T63	*Diethyl Zinc Mediated Metalloamination and Palladium Catalysis: Development and Application to the Synthesis of Functionalized Pyrrolidines and Piperidines*	Thomas Robinson, Montana State University Bryce Sunsdahl, Montana State University Tom Livinghouse, Montana State University Robert Szilagyi, Montana State University
T64	*The many particle expansion for systematic self interaction correction in DFT*	Tianyu Zhu, Massachusetts Institute of Technology Piotr de Silva, Massachusetts Institute of Technology Helen van Aggelen, Massachusetts Institute of Technology Troy Van Voorhis, Massachusetts Institute of Technology

T65	*Modeling Surface-Anchored Nematic Liquid Crystals for Chemoresponsive Applications*	Tibor Szilvasi University of Wisconsin-Madison Luke Roling, University of Wisconsin-Madison Huaizhe Yu, University of Wisconsin-Madison Prabin Rai, Kent State University Robert Twieg, Kent State University Nicholas Abbott, University of Wisconsin-Madison Manos Mavrikakis, University of Wisconsin-Madison
T66	*Confinement affect on the structural and dynamical properties of water in hydrophobic zeolites*	Tiecheng Zhou, Washington State University Aurora Clark, Washington State University
T67	*The Interplay of the Electronic Structure and Regioselectivity of C–H Bond Insertion of Nitrene Mediated by Dirutheium, Dirhodium, and Disilver Catalysts*	Tzuhsiung Yang, University of Wisconsin-Madison Adrian Varela-Alvarez, Emory University Djamaladdin Musaev, Emory University John Berry, University of Wisconsin-Madison
T68	*Gas phase modeling approach of excited state deactivation in model proteins chains*	Thibaut Very, DRF/IRAMIS/LYDYL UMR 9222 - LCPQ UMR Valarie Brenner, DRF/IRAMIS/LIDYL UMR
T69	*Comparative analysis of the structural determinants of endogeneous cannabinoids and activity of illicit drugs on Cannabinoid receptors type2*	Vivek Yadav, Temple University Khaled Elokely, Tanta University Michael Klein, Temple University
T70	*Efficient and Accurate Excited State Quantum Dynamics in Atomistic Condensed Phase Systems using Quantum-Classical Theory with Generalized Quantum Master Equations*	William Pfalzgraff, Department of Chemistry, Stanford University Aaron Kelly, Department of Chemistry, Stanford University Thomas Markland, Department of Chemistry, Stanford University
T71	*AARON: An Automated Reaction Optimizer for Non-metal catalyzed reactions*	Yanfei Guan, Department of Chemistry, Texas A&M University Steven E. Wheeler, Texas A&M University
T72	*Efficient graph-based method for finding reaction pathways through stochastic and deterministic intermediate samplings*	Yeonjoon Kim, Department of Chemistry, KAIST Sunghwan Choi, Department of Chemistry, KAIST Jin Woo Kim, Department of Chemistry, KAIST Zeehyo Kim, Department of Chemistry, KAIST Woo Youn Kim, Department of Chemistry, KAIST
T73	*Design of Ferromagnetic Organic Magnetic Materials: Doping on Graphene Nanoribbon, Terminated with Organic Radicals*	Yeonsig Nam, Sungkyunkwan University Daeheum Cho, Sungkyunkwan University Jin Yong Lee, Sungkyunkwan University
T74	*Can we decipher the mechanism for singlet fission in polyacene aggregates using density functional theory (DFT) based approaches?*	Zhou Lin, Department of Chemistry, Massachusetts Institute of Technology Troy Van Voorhis, Department of Chemistry, Massachusetts Institute of Technology
T75	*Photophysics of Bimanes*	Zi Cheng Wong, National University of Singapore Wai Yip Fan, National University of Singapore Tsz Sian Chwee, Institute of High Performance Computing Michael Sullivan, Institute of High Performance Computing