

Hai-Lung Dai Festschrift

Virtual Special Issue

Isolated Molecules, Clusters, Radicals, and Ions; Environmental Chemistry, Geochemistry, and Astrochemistry; New Tools and Methods		
Quantum Spin–Orbit Electronic State Selection of Atomic Transition Metal Vanadium Cation for Chemical Reactivity Studies	Yih Chung Chang, Bo Xiong, Yuntao Xu, Cheuk-Yiu Ng	10.1021/acs.jpca.9b00511
$A^2\Pi_u$ and $1^4\Sigma_u^-$ States of Br_2^+ Studied by [1+1] Two-Photon Dissociation Spectroscopy in a Cold Ion Beam	Hao Liang, Zhengfang Zhou, Zefeng Hua, Yunxiao Zhao, Shaowen Feng, Yang Chen, Dongfeng Zhao	10.1021/acs.jpca.9b03211
Odd–Even Reactivity Variation Due to Dynamical Effects around the Roaming Saddle Points of the Reaction Between C_n^- Chain ($n = 2\text{--}8$) and H_2	Daisuke Yoshida, Kaito Takahashi	10.1021/acs.jpca.9b03435
$\text{Re}\text{C}\text{B}_8^-$ and $\text{Re}\text{C}\text{B}_9^-$: New Members of the Transition-Metal-Centered Borometallic Molecular Wheel Family	Teng-Teng Chen, Wan-Lu Li, Hui Bai, Wei-Jia Chen, Xin-Ran Dong, Jun Li, Lai-Sheng Wang	10.1021/acs.jpca.9b03942
Competition between Proton Transfer and Proton Isomerization in the $\text{N}_2 + \text{HOC}^+$ Reaction on an <i>Ab Initio</i> -Based Global Potential Energy Surface	Qian Yao, Changjian Xie, Hua Guo	10.1021/acs.jpca.9b04115
Cation Vibrations of 1-Methylnaphthalene and 2-Methylnaphthalene through Mass-Analyzed Threshold Ionization Spectroscopy	Sheng Yuan Tzeng, Vidya S. Shivhare, Wen Bih Tzeng	10.1021/acs.jpca.9b03756
Infrared Emission from Photodissociation of Methyl Formate [HC(O)OCH_3] at 248 and 193 nm: Absence of Roaming Signature	Lucia Lanfri, Yen-Lin Wang, Tien V. Pham, Nghia Trong Nguyen, Maxi Burgos Paci, M. C. Lin, Yuan-Pern Lee	10.1021/acs.jpca.9b04129
Interfaces of Gas–Aerosol Particles: Relative Humidity and Salt Concentration Effects	Yuqin Qian, Gang-hua Deng, Jordan Lapp, Yi Rao	10.1021/acs.jpca.9b03896
Formation of Copper(I) Oxide- and Copper(I) Cyanide–Polyacetonitrile Nanocomposites through Strong-Field Laser Processing of Acetonitrile Solutions of Copper(II) Acetate Dimer	Behzad Tangeysh, Johanan H. Odhner, Yu Wang, Bradford B. Wayland, Robert J. Levis	10.1021/acs.jpca.9b04206
Ultrafast Excited-State Intermolecular Proton Transfer in Indigo Oligomer	Xuemei He, Fan Yang, Shuang Li, Xiaoxiao He, Anchi Yu, Jinquan Chen, Jianhua Xu, Jianping Wang	10.1021/acs.jpca.9b06427
Hydrogen-Bonding Motifs and Proton-Transfer Dynamics in Electronically Excited 6-Hydroxy-2-formylfulvene	Zachary N. Vealey, Lidor Foguel, Patrick H. Vaccaro	10.1021/acs.jpca.9b05025

Molecular Dynamics Simulation of Zinc Ion in Water with an ab Initio Based Neural Network Potential	Mingyuan Xu, Tong Zhu, John Z. H. Zhang	10.1021/acs.jpca.9b04087
Stereodynamic Imaging of Bromine Atomic Photofragments Eliminated from 1-Bromo-2-methylbutane Oriented via Hexapole State Selector	Masaaki Nakamura, Hsiu-Pu Chang, King-Chuen Lin, Toshio Kasai, Dock-Chil Che, Federico Palazzetti, Vincenzo Aquilanti	10.1021/acs.jpca.9b04048
Toward Closing the Gap between Hexoses and <i>N</i> -Acetylhexosamines: Experimental and Computational Studies on the Collision-Induced Dissociation of Hexosamines	Cheng-chau Chiu, Hai Thi Huynh, Shang-Ting Tsai, Hou-Yu Lin, Po-Jen Hsu, Huu Trong Phan, Arya Karumanthra, Hayden Thompson, Yu-Chi Lee, Jer-Lai Kuo, Chi-Kung Ni	10.1021/acs.jpca.9b04143
Direct Dynamics Simulations of Fragmentation of a Zn(II)-2Cys-2His Oligopeptide. Comparison with Mass Spectrometry Collision-Induced Dissociation	Abdul Malik, Yu-Fu Lin, Subha Pratihar, Laurence A. Angel, William L. Hase	10.1021/acs.jpca.9b05218
Collisional Energy Transfer from vibrationally Excited Hydrogen Isocyanide	Michael J. Wilhelm, Hai-Lung Dai	10.1021/acs.jpca.9b07041
Extracting Information on Linear and Nonlinear Absorption from Two-Beam Action Spectroscopy Data	Samuel R. Cohen, John T. Fourkas	10.1021/acs.jpca.9b06068
Chemistry and Photochemistry of Pyruvic Acid Adsorbed on Oxide Surfaces	Michael R. Alves, Yuan Fang, Kristin J. Wall, Veronica Vaida, Vicki H. Grassian	10.1021/acs.jpca.9b06563
Machine Learning for Predicting Electron Transfer Coupling	Chun-I Wang, Mac Kevin E. Braza, Gil C. Claudio, Ricky B. Nellas, Chao-Ping Hsu	10.1021/acs.jpca.9b04256
Biophysics, Biomaterials, Liquids, Soft Matter		
Exposing the Nucleation Site in α -Helix Folding: A Joint Experimental and Simulation Study	Arusha Acharyya, Yunhui Ge, Haifan Wu, William F. DeGrado, Vincent A. Voelz, Feng Gai	10.1021/acs.jpcb.8b12220
Understanding the Dynamic Behavior of an Anticancer Drug, Doxorubicin, on a Lipid Membrane Using Multiple Spectroscopic Techniques	Yi Hou, Shun-Li Chen, Wei Gan, Xing Ma, Qunhui Yuan	10.1021/acs.jpcb.9b01941
Bacterial Model Membranes Deform (<i>resp.</i> Persist) upon Ni^{2+} Binding to Inner Core (<i>resp.</i> O-Antigen) of Lipopolysaccharides	HanByul Chang, Karthikeyan Gnanasekaran, Nathan C. Gianneschi, Franz M. Geiger	10.1021/acs.jpcb.9b02762
Polarized Two-Photon Absorption and Heterogeneous Fluorescence Dynamics in NAD(P)H	Thomas S. Blacker, Nick Nicolaou, Michael R. Duchen, Angus J. Bain	10.1021/acs.jpcb.9b01236
Ultrafast Hydrogen Bond Exchanging between Water and Anions in Concentrated Ionic Liquid Aqueous Solutions	Qianshun Wei, Miaomiao Zhang, Dexia Zhou, Xiaoqian Li, Hongtao Bian, Yu Fang	10.1021/acs.jpcb.9b03504

Nitration of Tyrosine Channels Photoenergy through a Conical Intersection in Water	Longteng Tang, Chong Fang	10.1021/acs.jpcb.9b03464
3D Tracking-Free Approach for Obtaining 3D Super-Resolution Information in Rotationally Symmetric Biostructures	Andrew Ruba, Wangxi Luo, Joseph Kelich, Mark Tingey, Weidong Yang	10.1021/acs.jpcb.9b02979
Dynamic Heterogeneities in Colloidal Supercooled Liquids: Experimental Tests of Inhomogeneous Mode Coupling Theory	Chandan K. Mishra, Piotr Habdas, A. G. Yodh	10.1021/acs.jpcb.9b03419
Comparison and Elucidation of Structural Diversity and Variation of G-Rich Sequences with a Single G-Base Difference	I-Te Chu, Ting-Yuan Tseng, Ta-Chau Chang	10.1021/acs.jpcb.9b02956
Chiral Inversion of Amino Acids in Antiparallel β -Sheets at Interfaces Probed by Vibrational Sum Frequency Generation Spectroscopy	Ethan A. Perets, Pablo E. Videla, Elsa C. Y. Yan, Victor S. Batista	10.1021/acs.jpcb.9b04029
Pressure Effects on Protein Hydration Water Thermodynamics	Viren Pattni, Matthias Heyden	10.1021/acs.jpcb.9b04094
Modulation of Surface-Catalyzed Secondary Nucleation during Amyloid Fibrillation of Hen Egg White Lysozyme by Two Common Surfactants	Yao Wang, Baohuan Jia, Min You, Haoran Fan, Siyu Cao, Hui Li, Wenkai Zhang, Gang Ma	10.1021/acs.jpcb.9b04036
Local Ordering of Lattice Self-Assembled SDS@2 β -CD Materials and Adsorbed Water Revealed by Vibrational Sum Frequency Generation Microscope	Haoyuan Wang, Wenfan Chen, Jackson C. Wagner, Wei Xiong	10.1021/acs.jpcb.9b04928
Characterization of Single-Protein Dynamics in Polymer-Cushioned Lipid Bilayers Derived from Cell Plasma Membranes	Wai Cheng Wong, Jz-Yuan Juo, Chih-Hsiang Lin, Yi-Hung Liao, Ching-Ya Cheng, Chia-Lung Hsieh	10.1021/acs.jpcb.9b03789
Mueller Tensor Nonlinear Optical Polarization Analysis in Turbid Media	James R.W. Ulcickas, Garth J. Simpson	10.1021/acs.jpcb.9b04961
Temperature Dependence of the Energy Transfer in LHCII Studied by Two-Dimensional Electronic Spectroscopy	Parveen Akhtar, Thanh Nhut Do, Paweł J. Nowakowski, Adriana Huerta-Viga, M. Faisal Khyasudeen, Petar H. Lambrev, Howe-Siang Tan	10.1021/acs.jpcb.9b05421
Smart Hybrid Nanocomposite for Photodynamic Inactivation of Cancer Cells with Selectivity	Jeong-Wook Hwang, Seung-Jin Jung, Taek-Chin Cheong, Yuri Kim, Eon Pil Shin, Il Heo, Gwanghun Kim, Nam-Hyuk Cho, Kang-Kyun Wang, Yong-Rok Kim	10.1021/acs.jpcb.9b04301
Surface Topography Effects of Globular Biomolecules on Hydration Water	Sheh-Yi Sheu, Yu-Cheng Liu, Jia-Kai Zhou, Edward W. Schlag, Dah-Yen Yang	10.1021/acs.jpcb.9b03734
A Novel Method to Measure the Effective Change of the Interfacial	Yi-Chih Lin, Murray Skolnick, Zahra Fakhraai	10.1021/acs.jpcb.9b04717

Energy due to Kinetic Self-Assembly of Amyloid Fibrils		
Photodynamics of [FeFe]-Hydrogenase Model Compounds with Bidentate Heterocyclic Ligands	Wyatt Thornley, Sarah A. Wirick, Maximilian Riedel-Topper, Nathan J. DeYonker, Thomas E. Bitterwolf, Christopher J. Stromberg, Edwin J. Heilweil	10.1021/acs.jpcb.9b04675
Determination of the Rate-Limiting Step in Fatty Acid Transport	Victoria Cheng, Dylan R. Kimball, Dr. John C. Conboy	10.1021/acs.jpcb.9b05162
Theoretical Investigation of Positional Substitution and Solvent Effects on <i>n</i> -Cyanoindole Fluorescent Probes	Salsabil Abou-Hatab, Spiridoula Matsika	10.1021/acs.jpcb.9b05961
Molecular Adsorption and Transport at Liposome Surfaces Studied by Molecular Dynamics Simulations and Second Harmonic Generation Spectroscopy	Prakash Hamal, Huy Nguyenhuu, Visal Subasinghe Don, Raju R. Kumal, Revati Kumar, Robin L. McCarley, Louis H. Haber	10.1021/acs.jpcb.9b05954
Energy Conversion and Storage; Catalysis; Optical, Electronic, and Magnetic Properties and Processes; Interfaces; Nanomaterials and Hybrid Materials		
Effect of Functional and Electron Correlation on the Structure and Spectroscopy of the Al ₂ O ₃ (001)–H ₂ O Interface	Mark J. DelloStritto, Stefan M. Piontek, Michael L. Klein, Eric Borguet	10.1021/acs.jpcllett.9b00016
Understanding the Diverse Coordination Modes of Thiocyanate Anion on Solid Surfaces	Zheng Wang, Tongfa Liu, Xia Long, Yuan Li, Fuquan Bai, Shihe Yang	10.1021/acs.jpcc.9b01457
Laser Synthesis and Spectroscopy of Molybdenum Oxide Nanorods	Melissa P. Woodard, Michael A. Duncan	10.1021/acs.jpcc.9b00627
Dicopper Dioxygenase Model Immobilized in Mesoporous Silica Nanoparticles for Toluene Oxidation: A Mechanism to Harness Both O Atoms of O ₂ for Catalysis	Chih-Cheng Liu, Yi-Fang Tsai, Chung-Yuan Mou, Steve S.-F. Yu, Sunney I. Chan	10.1021/acs.jpcc.9b02508
Suppression of Defect-Induced Quenching via Chemical Potential Tuning: A Theoretical Solution for Enhancing Lanthanide Luminescence	Xian Qin, Lei Shen, Liangliang Liang, Sanyang Han, Zhigao Yi, Xiaogang Liu	10.1021/acs.jpcc.9b02596
Cooperative Action of Laser-Induced Thermal Effects and Ionic Coordination on the Order of TPPA0 Porphyrin Derivatives Self-Assembled Interface Probed via Real-Time Second Harmonic Generation	Bin Dong, Ruipeng Bai, Wuming Zheng, Man Xue, Caihe Liu, Minghua Liu, Zhen Zhang, Yuan Guo	10.1021/acs.jpcc.9b03165
Photochemical Synthesis of Azoarenes from Aryl Azides on Cu(100): A Mechanism Unraveled	Yun-Wen Luo, Chih-Hung Chou, Po-Chiao Lin, Chao-Ming Chiang	10.1021/acs.jpcc.8b12373
Interaction of Gold with Oxide Nanoparticles: Size or Electronic Effect?	Oleksandr Bondarchuk, Shamil Shaikhutdinov, Hans-Joachim Freund	10.1021/acs.jpcc.9b02592

Effect of an External Electric Field on the Fluorescence of a π -Conjugated Polymer Film of P3HT Sandwiched between FTO and PMMA	Kamlesh Awasthi, Chin-Shiun Chiou, Toshifumi Iimori, Eric Wei-Guang Diau, Nobuhiro Ohta	10.1021/acs.jpcc.9b02946
Toward Unraveling the Puzzle of Sum Frequency Generation Spectra at Interface of Aqueous Methanol Solution: Effects of Concentration-Dependent Hyperpolarizability	Xia Li, Jianchuan Liu, Ke Lin, Yun Zhang, Yunhong Zhang, Renhui Zheng, Qiang Shi, Yuan Guo, Zhou Lu	10.1021/acs.jpcc.9b04044
Effect of Interlayer Co^{2+} on Structure and Charge Transfer in NiFe Layered Double Hydroxides	Mark J. DelloStritto, Akila C. Thenuwara, Michael L. Klein, Daniel R. Strongin	10.1021/acs.jpcc.9b01671
Rapid Bimolecular and Defect-Assisted Carrier Recombination in Hexagonal Boron Nitride	Ioannis Chatzakis, Roderick B. Davidson, Adam D. Dunkelberger, Song Liu, Jaime Freitas, James Culbertson, J. H. Edgar, Daniel C. Ratchford, Chase T. Ellis, Andrea B. Grafton, Alexander J. Giles, Joseph G. Tischler, Joshua D. Caldwell, Jeffrey C. Wrutsky	10.1021/acs.jpcc.9b04118
Bimodal Bandgaps in Mixed Cesium Methylammonium Lead Bromide Perovskite Single Crystals	Fang Liu, Feifan Wang, Kameron R. Hansen, X.-Y. Zhu	10.1021/acs.jpcc.9b03536
α -Quartz Crystal as Absolute Intensity and Phase Standard in Sum-Frequency Generation Vibrational Spectroscopy	Xiao-Hua Hu, Feng Wei, Hui Wang, Hong-Fei Wang	10.1021/acs.jpcc.9b03202
All-Optical Thermometry with Nitrogen-Vacancy Centers in Nanodiamond-Embedded Polymer Films	Yuen Yung Hui, Oliver Y. Chen, Terumitsu Azuma, Be-Ming Chang, Feng-Jen Hsieh, Huan-Cheng Chang	10.1021/acs.jpcc.9b04496
Sodium Halide Adsorption and Water Structure at the α -Alumina(0001)/Water Interface	Ruiyu Wang, Mark DelloStritto, Richard C. Remsing, Vincenzo Carnevale, Michael L. Klein, Eric Borguet	10.1021/acs.jpcc.9b03054
Quantum Monte Carlo Studies of CO Adsorption on Transition Metal Surfaces	Cheng-Rong Hsing, Chun-Ming Chang, Ching Cheng, Ching-Ming Wei	10.1021/acs.jpcc.9b03780
Effect of Frequency-Dependent Fresnel Factor on the Vibrational Sum Frequency Generation Spectra for Liquid/Solid Interfaces	Lin Wang, Satoshi Nihonyanagi, Ken-ichi Inoue, Kei Nishikawa, Akihiro Morita, Shen Ye, Tahei Tahara	10.1021/acs.jpcc.9b04043
Light-Like Group Velocities and Long Lifetimes for Leaky Surface Plasmon Polaritons in Noble Metal Nanostripes	Gary Beane, Brendan S. Brown, Tuphan Devkota, Gregory V. Hartland	10.1021/acs.jpcc.9b03001
Spin-Crossover and Coherent Transport Behaviors of a Six-Coordinate Iron(II) Complex with a N_4O_2 Donor Set	Yue Gu, Yujie Hu, Jing Huang, Qunxiang Li, Jinlong Yang	10.1021/acs.jpcc.9b02856
Anchoring of Aminophosphonates on Titanium Oxide for Biomolecular Coupling	Paolo Canepa, Grazia Gonella, Giulia Pinto, Vladimir Grachev, Maurizio Canepa, Ornella Cavalleri	10.1021/acs.jpcc.9b04077

Sticking Probability of High-Energy Methane on Crystalline, Amorphous, and Porous Amorphous Ice Films	Rebecca S. Thompson, Michelle R. Brann, S. J. Sibener	10.1021/acs.jpcc.9b03900
Monovalent and Divalent Cations at the α -Al ₂ O ₃ (0001)/Water Interface: How Cation Identity Affects Interfacial Ordering and Vibrational Dynamics	Stefan M. Piontek, Aashish Tuladhar, Tim Marshall, Eric Borguet	10.1021/acs.jpcc.9b01618
Thermal Atomic Layer Etching of Al ₂ O ₃ , HfO ₂ , and ZrO ₂ Using Sequential Hydrogen Fluoride and Dimethylaluminum Chloride Exposures	Younghlee Lee, Steven M. George	10.1021/acs.jpcc.9b04767
Mesoporous Silica Nanospheres Decorated by Ag–Nanoparticle Arrays with 5 nm Interparticle Gap Exhibit Insignificant Hot-Spot Raman Enhancing Effect	Wan-Tzu Chen, Yu-Wei Cheng, Ming-Chien Yang, Ru-Jong Jeng, Ting-Yu Liu, Juen-Kai Wang, Yuh-Lin Wang	10.1021/acs.jpcc.9b04074
Determining the Spheroid Geometry of Individual Metallic Nanoparticles by Two-Dimensional Single-Particle Dynamic Light Scattering	Luis F. Guerra, Tom W. Muir, Haw Yang	10.1021/acs.jpcc.9b05217
Ligand Dependent Growth and Optical Properties of Hybrid Organo-metal Halide Perovskite Magic Sized Clusters	Evan T. Vickers, Ke Xu, Benjamin W. Dreskin, Thomas A. Graham, Xueming Li, Jin Z. Zhang	10.1021/acs.jpcc.9b05521
Fabrication of Anisotropic Silver Nanoplatelets on the Surface of TiO ₂ Fibers for Enhanced Photocatalysis of a Chemical Warfare Agent Simulant, Methyl Paraoxon	Danielle L. Kuhn, Zachary Zander, Ann M. Kulisiwicz, S. M. Debow, Connor Haffey, Hui Fang, Xiang-Tian Kong, Yuqin Qian, Scott D. Walck, Alexander O. Govorov, Yi Rao, Hai-Lung Dai, Brendan G. DeLacy	10.1021/acs.jpcc.9b04026
Capturing the Long-Lived Photogenerated Electrons in Au/TiO ₂ upon UV or Visible Irradiation by Time-Resolved Infrared Spectroscopy	Xiaojuan Dai, Zeqing Jiao, Zehan Ma, Kunhui Liu, Chen Wang, Hongmei Su	10.1021/acs.jpcc.9b05096
Surface Characterization of Colloidal Silica Nanoparticles by Second Harmonic Scattering: Quantifying the Surface Potential and Interfacial Water Order	Arianna Marchioro, Marie Bischoff, Cornelis Lütgebaucks, Denys Biriukov, Milan Předota, Sylvie Roke	10.1021/acs.jpcc.9b05482
Effect of Surface Ligand on Charge Separation and Recombination at CsPbI ₃ Perovskite Quantum Dot/TiO ₂ Interfaces	Qiongyi Shang, Brandon D. Piercy, Mark D. Losego, Tianquan Lian	10.1021/acs.jpcc.9b06725
Comparative Study of the Adsorption of Thiol and Isocyanide Molecules on a Silver Surface by in Situ Surface-Enhanced Raman Scattering	Jaewan Ahn, Shi Shi, Bonnie Vannatter, Dong Qin	10.1021/acs.jpcc.9b05383
Probing the Interfacial Symmetry Using Rotational Second-Harmonic Generation in Oxide Heterostructures	Kun Zhao, Joel E. Taylor, Louis H. Haber, Jiandi Zhang, E. W. Plummer, Mohammad Saghayezhian	10.1021/acs.jpcc.9b05974