

100  
J80/pa

SEPTEMBER 4, 2014

VOLUME 118

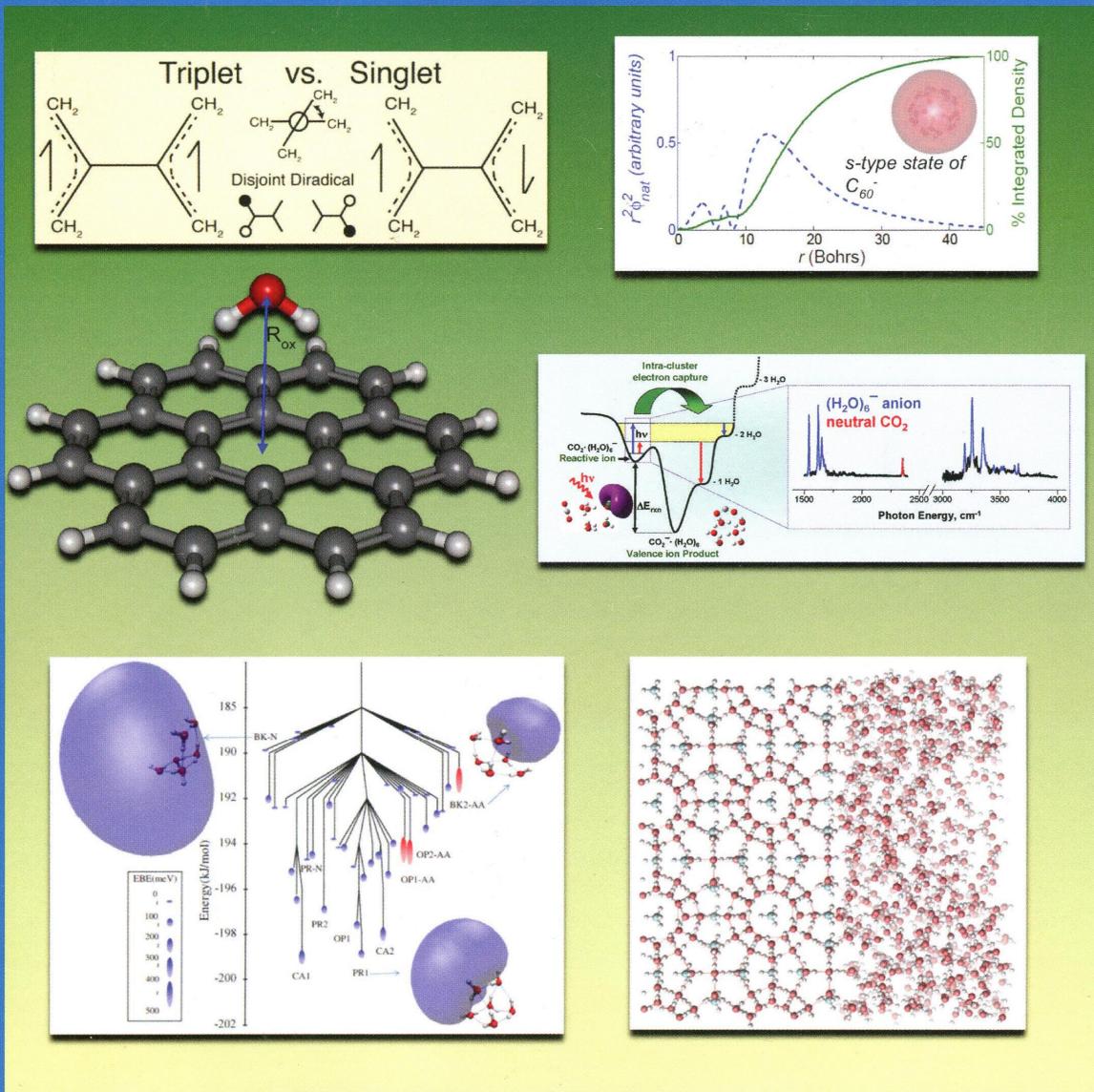
NUMBER 35

[pubs.acs.org/JPCA](http://pubs.acs.org/JPCA)

# THE JOURNAL OF PHYSICAL CHEMISTRY

A

**Collage of Figures  
Representing Research  
Projects Undertaken  
in the Jordan  
Research Group  
(see page 5A)**



## KENNETH D. JORDAN FESTSCHRIFT



**ACS Publications**  
Most Trusted. Most Cited. Most Read.

[www.acs.org](http://www.acs.org)

**ON THE COVER:** Collage of artwork adapted from Jordan papers. (Upper left) Pozun, Z. D.; Su, X.; Jordan, K. D. Establishing the Ground State of the Disjoint Diradical Tetramethyleneethane with Quantum Monte Carlo. *J. Am. Chem. Soc.* **2013**, *135*, 13862–13869. (Upper right) Voora, V.; Cederbaum, L. S.; Jordan, K. D. Existence of a Correlation Bound *s*-Type Anion State of  $C_{60}$ . *J. Phys. Chem. Lett.* **2013**, *4*, 849–853. (Middle left) For details see Jenness G.; Jordan K. D. A DF-DFT-SAPT Investigation of the Binding of Water of Coronene and Dodecabenzenocoronene: Implications for the Water–Graphite Interaction. *J. Phys. Chem. B*, **2009**, *113*, 10242–10248. (Middle right) Breen, J.; DeBlase, A. F.; Guasco, T. L.; Voora, V. K.; Jordan, K. D.; Nagata, T.; Johnson, M. A. A Bottom-up View of Water Network-Mediated  $CO_2$  Reduction using Cryogenic Cluster Ion Spectroscopy and Direct Dynamics Simulations. *J. Phys. Chem. A*, **2012**, *116*, 903–9012. (Lower left) Reprinted from Choi T.-H.; Jordan, K. D. Potential Energy Landscape of the  $(H_2O)_6$ -Cluster. *Chem. Phys. Lett.*, **2009**, *475*, 293–297 with permission from Elsevier. (Lower right) Myshakin, E.; Jiang, H.; Warzinski, R.; Jordan, K. D. Molecular Dynamics Simulations of Methane Hydrate Decomposition. *J. Phys. Chem. A*, **2009**, *113*, 1913–1921. This special issue was organized by Guest Editors: Mark Johnson, Jack Simons, and Feng Wang.

## SPECIAL ISSUE: KENNETH D. JORDAN FESTSCHRIFT

Guest Editors: Mark Johnson, Jack Simons, and Feng Wang

### Special Issue Preface

7167

[dx.doi.org/10.1021/jp500588d](https://doi.org/10.1021/jp500588d)

From Quantum Mechanics to Molecular Mechanics: A Tribute to Kenneth D. Jordan  
Mark Johnson, Jack Simons, and Feng Wang\*

7169

[dx.doi.org/10.1021/jp409886k](https://doi.org/10.1021/jp409886k)

Autobiography of Kenneth D. Jordan

7172

[dx.doi.org/10.1021/jp409885g](https://doi.org/10.1021/jp409885g)

Colleagues of Kenneth D. Jordan

7174

[dx.doi.org/10.1021/jp500584b](https://doi.org/10.1021/jp500584b)

Curriculum Vitae of Kenneth D. Jordan

7175

[dx.doi.org/10.1021/jp5005852](https://doi.org/10.1021/jp5005852)

Publications of Kenneth D. Jordan

## Articles

7186

[dx.doi.org/10.1021/jp405910k](https://doi.org/10.1021/jp405910k)

Computational Studies of [bmim][PF<sub>6</sub>]/*n*-Alcohol Interfaces with Many-Body Potentials  
Tsun-Mei Chang\* and Liem X. Dang\*

7194

[dx.doi.org/10.1021/jp411666a](https://doi.org/10.1021/jp411666a)

**Prediction of Thymine Dimer Repair by Electron Transfer from Photoexcited 8-Aminoguanine or Its Deprotonated Anion**  
Iwona Sieradzan, Marzena Marchaj, Iwona Anusiewicz, Piotr Skurski, and Jack Simons\*

7201

[dx.doi.org/10.1021/jp408386f](https://doi.org/10.1021/jp408386f)

**Nonvalence Correlation-Bound Anion State of C<sub>6</sub>F<sub>6</sub>: Doorway to Low-Energy Electron Capture**  
Vamsee K. Voora and Kenneth D. Jordan\*

7206

[dx.doi.org/10.1021/jp408821a](https://doi.org/10.1021/jp408821a)

**Simultaneous Evaluation of Multiple Rotationally Excited States of H<sub>3</sub><sup>+</sup>, H<sub>3</sub>O<sup>+</sup>, and CH<sub>5</sub><sup>+</sup> Using Diffusion Monte Carlo**  
Andrew S. Petit, Jason E. Ford, and Anne B. McCoy\*

7221

[dx.doi.org/10.1021/jp408913k](https://doi.org/10.1021/jp408913k)

**Multistate Treatments of the Electronic Coupling in Donor–Bridge–Acceptor Systems: Insights and Caveats from a Simple Model**  
Robert J. Cave\* and Marshall D. Newton\*

7235

[dx.doi.org/10.1021/jp409209s](https://doi.org/10.1021/jp409209s)

**Effects of Topological Defects and Diatom Vacancies on Characteristic Vibration Modes and Raman Intensities of Zigzag Single-Walled Carbon Nanotubes**  
Wissam A. Saidi\*

7242

[dx.doi.org/10.1021/jp409345m](https://doi.org/10.1021/jp409345m)

**Temporary Anion States of Three Herbicide Families**  
A. M. Scheer, K. Aflatoonni, G. A. Gallup, and P. D. Burrow\*

7249

[dx.doi.org/10.1021/jp4104596](https://doi.org/10.1021/jp4104596)

**Photoelectron Angular Distributions as Probes of Cluster Anion Structure: I<sup>-</sup>(H<sub>2</sub>O)<sub>2</sub> and I<sup>-</sup>(CH<sub>3</sub>CN)<sub>2</sub>**  
Foster Mbaiwa, Nicholas Holtgrewe, Diep Bich Dao, Joshua Lasinski, and Richard Mabbs\*

7255

[dx.doi.org/10.1021/jp410460m](https://doi.org/10.1021/jp410460m)

**Nonnuclear Nearly Free Electron Conduction Channels Induced by Doping Charge in Nanotube–Molecular Sheet Composites**  
Jin Zhao,\* Qijing Zheng, Hrvoje Petek,\* and Jinlong Yang\*

7261

[dx.doi.org/10.1021/jp410713d](https://doi.org/10.1021/jp410713d)

**Stability of Hemi-Bonded vs Proton-Transferred Structures of (H<sub>2</sub>O)<sub>2</sub><sup>+</sup>, (H<sub>2</sub>S)<sub>2</sub><sup>+</sup>, and (H<sub>2</sub>Se)<sub>2</sub><sup>+</sup> Studied with Projected Hartree–Fock Methods**  
Tamar Stein, Carlos A. Jiménez-Hoyos, and Gustavo E. Scuseria\*

7267

**Delicate Balance of Hydrogen Bonding Forces in *D*-Threonitol**

Vanesa Vaquero-Vara, Di Zhang, Brian C. Dian, David W. Pratt,\* and Timothy S. Zwier\*

[dx.doi.org/10.1021/jp410859n](https://doi.org/10.1021/jp410859n)

7274

[dx.doi.org/10.1021/jp410927a](https://doi.org/10.1021/jp410927a)**CO Capture and Conversion to HOCO Radical by Ionized Water Clusters**

Han Myoung Lee,\* Il-Seung Youn, and Kwang S. Kim\*

7280

[dx.doi.org/10.1021/jp411281y](https://doi.org/10.1021/jp411281y)**Communication Maps of Vibrational Energy Transport Through Photoactive Yellow Protein**

Yao Xu and David M. Leitner\*

7288

[dx.doi.org/10.1021/jp411294j](https://doi.org/10.1021/jp411294j)**Laser Multiphoton Ionization of Tetrakis(dimethylamino)ethylene**

Byron H. Smith and Robert N. Compton\*

7297

[dx.doi.org/10.1021/jp4115157](https://doi.org/10.1021/jp4115157)**Infrared Spectroscopy of Protonated Trimethylamine–(Benzene)<sub>n</sub> (*n* = 1–4) as Model Clusters of the Quaternary Ammonium–Aromatic Ring Interaction**

Ryunosuke Shishido, Yuki Kawai, and Asuka Fujii\*

7306

[dx.doi.org/10.1021/jp4115817](https://doi.org/10.1021/jp4115817)**Kinetic Monte Carlo Simulation of CO Adsorption on Sulfur-Covered Pd(100)**

Dominic R. Alfonso\*

7314

[dx.doi.org/10.1021/jp411681f](https://doi.org/10.1021/jp411681f)**A Nuclear Magnetic Resonance Study of the Binding of Trimethylphosphine Selenide to Cadmium Oleate**

Raúl García-Rodríguez and Haitao Liu\*

7320

[dx.doi.org/10.1021/jp411787w](https://doi.org/10.1021/jp411787w)**Excess Electrons Bound to Molecular Systems with a Vanishing Dipole but Large Molecular Quadrupole**

Thomas Sommerfeld,\* Katelyn M. Dreux, and Robin Joshi

7330

[dx.doi.org/10.1021/jp4118375](https://doi.org/10.1021/jp4118375)**Does Hydrophilicity of Carbon Particles Improve Their Ice Nucleation Ability?**

Laura Lupi and Valeria Molinero\*

7338

[dx.doi.org/10.1021/jp4119666](https://doi.org/10.1021/jp4119666)**Clusters of Coarse-Grained Water Molecules**

James D. Farrell\* and David J. Wales\*

7349

[dx.doi.org/10.1021/jp412055r](https://doi.org/10.1021/jp412055r)**Validation Challenge of Density-Functional Theory for Peptides—Example of Ac-Phe-Ala<sub>5</sub>-LysH<sup>+</sup>**

Mariana Rossi,\* Sucismita Chutia, Matthias Scheffler, and Volker Blum\*

7360

[dx.doi.org/10.1021/jp4121589](https://doi.org/10.1021/jp4121589)**Incorporation of ROH (R = CH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>, 2-C<sub>3</sub>H<sub>7</sub>) into (H<sub>2</sub>O)<sub>6</sub><sup>-</sup>: Substituent Effect on the Growth Process of the Hydrogen-Bond Network**

Ryuzo Nakanishi and Takashi Nagata\*

7367

[dx.doi.org/10.1021/jp412264t](https://doi.org/10.1021/jp412264t)**A New Many-Body Potential Energy Surface for HCl Clusters and Its Application to Anharmonic Spectroscopy and Vibration–Vibration Energy Transfer in the HCl Trimer**

John S. Mancini and Joel M. Bowman\*

7375

[dx.doi.org/10.1021/jp4123997](https://doi.org/10.1021/jp4123997)**Stabilization of a Cl<sup>-</sup>–Cl<sup>-</sup> Anion Pair in the Gas Phase: Ab Initio Microsolvation Study**

Alexander S. Ivanov, Gernot Frenking,\* and Alexander I. Boldyrev\*

7385

[dx.doi.org/10.1021/jp4125638](https://doi.org/10.1021/jp4125638)**Intermolecular Interactions between Molecules in Various Conformational States: The Dimer of Oxalic Acid**

Zibo G. Keolopile,\* Matthew R. Ryder,\* and Maciej Gutowski\*

7392

[dx.doi.org/10.1021/jp412727w](https://doi.org/10.1021/jp412727w)**Accurate Bond Energies of Biodiesel Methyl Esters from Multireference Averaged Coupled-Pair Functional Calculations**

Victor B. Oyeyemi, John A. Keith, and Emily A. Carter\*

7404

[dx.doi.org/10.1021/jp412740j](https://doi.org/10.1021/jp412740j)**Piezoelectric Hydrogen Bonding: Computational Screening for a Design Rationale**

Keith A. Werling, Maryanne Griffin, Geoffrey R. Hutchison, and Daniel S. Lambrecht\*

7411

[dx.doi.org/10.1021/jp412779q](https://doi.org/10.1021/jp412779q)**Sorption of H<sub>2</sub> to Open Metal Sites in a Metal–Organic Framework: A Symmetry-Adapted Perturbation Theory Analysis**

Joshua J. Goings, Suzanna M. Ohlsen, Kara M. Blaisdell, and Daniel P. Schofield\*

7418

[dx.doi.org/10.1021/jp412816w](https://doi.org/10.1021/jp412816w)**C vs N: Which End of the Cyanide Anion Is a Better Hydrogen Bond Acceptor?**

Raghunath O. Ramabhadran, Yuran Hua, Amar H. Flood, and Krishnan Raghavachari\*

7424

**Electron Propagator Calculations on the Ground and Excited States of C<sub>60</sub>**  
V. G. Zakrzewski, O. Dolgounitcheva, and J. V. Ortiz\*

[dx.doi.org/10.1021/jp412813m](https://doi.org/10.1021/jp412813m)

7430



**Hydration of the Sulfuric Acid–Methylamine Complex and Implications for Aerosol Formation**  
Danielle J. Bustos, Berhane Temelso, and George C. Shields\*

[dx.doi.org/10.1021/jp500015t](https://doi.org/10.1021/jp500015t)

7442



**Calculation of Iron Transport through Human H-chain Ferritin**  
Rozita Laghaei, William Kowallis, Deborah G. Evans, and Rob D. Coalson\*

[dx.doi.org/10.1021/jp500198u](https://doi.org/10.1021/jp500198u)

7454



**Molecular Dynamics Simulations of Turbostratic Dry and Hydrated Montmorillonite with Intercalated Carbon Dioxide**  
Evgeniy M. Myshakin,\* Meysam Makaremi, Vyacheslav N. Romanov, Kenneth D. Jordan, and George D. Guthrie

[dx.doi.org/10.1021/jp500221w](https://doi.org/10.1021/jp500221w)

7469



**Ab Initio Thermodynamic Model for Magnesium Carbonates and Hydrates**  
Anne M. Chaka\* and Andrew R. Felmy

[dx.doi.org/10.1021/jp500271n](https://doi.org/10.1021/jp500271n)

7489

**Assessment of Various Electronic Structure Methods for Characterizing Temporary Anion States: Application to the Ground State Anions of N<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>4</sub>H<sub>6</sub>**  
Michael F. Falsetta,\* Laura A. DiFalco, Daniel S. Ackerman, John C. Barlow, and Kenneth D. Jordan

[dx.doi.org/10.1021/jp5003287](https://doi.org/10.1021/jp5003287)

7498



**Static Density Functional Study of Graphene–Hexagonal Bilayer Ice Interaction**  
David J. Anick

[dx.doi.org/10.1021/jp500360n](https://doi.org/10.1021/jp500360n)

7507



**Optical Spectroscopy of the Bulk and Interfacial Hydrated Electron from Ab Initio Calculations**  
Frank Uhlig, John M. Herbert,\* Marc P. Coons, and Pavel Jungwirth\*

[dx.doi.org/10.1021/jp5004243](https://doi.org/10.1021/jp5004243)

7516



**Coordination versus Solvation in Al<sup>+</sup>(benzene)<sub>n</sub> Complexes Studied with Infrared Spectroscopy**  
Kimberly N. Reishus, Antonio D. Brathwaite, Jonathan D. Mosley, and Michael A. Duncan\*

[dx.doi.org/10.1021/jp500778w](https://doi.org/10.1021/jp500778w)

- 7526 dx.doi.org/10.1021/jp501089n  
**Computational Investigation of the Lewis Acidity in Three-Dimensional and Corresponding Two-Dimensional Zeolites: UTL vs IPC-1P**  
Ho Viet Thang, Miroslav Rubeš, Ota Bludský, and Petr Nachtigall\*
- 7535 dx.doi.org/10.1021/jp501094n  
**Spectroscopic Properties of Benzene at the Air–Ice Interface: A Combined Experimental–Computational Approach**  
Rafał Kania, Joseph K'Eküboni Malongwe, Dana Nachtigallová,\* Ján Krausko, Ivan Gladich, Martina Roeselová, Dominik Heger,\* and Petr Klán\*
- 7548 dx.doi.org/10.1021/jp5015498  
**Renormalized Coupled Cluster Approaches in the Cluster-in-Molecule Framework: Predicting Vertical Electron Binding Energies of the Anionic Water Clusters ( $\text{H}_2\text{O}$ )<sub>n</sub><sup>-</sup>**  
Peng Xu and Mark S. Gordon\*
- 7560 dx.doi.org/10.1021/jp502282v  
**Twisted Triplet Ethylene: Anharmonic Frequencies and Spectroscopic Parameters for  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{D}_4$ , and  $^{13}\text{C}_2\text{H}_4$**   
Xiao Wang, Walter E. Turner II, Jay Agarwal, and Henry F. Schaefer III\*
- 7568 dx.doi.org/10.1021/jp5024235  
**Benchmark Theoretical Study of the  $\pi$ – $\pi$  Binding Energy in the Benzene Dimer**  
Evangelos Miliordos, Edoardo Aprà, and Sotiris S. Xantheas\*
- 7579 dx.doi.org/10.1021/jp502826e  
**A Three-Step Kinetic Model for Electrochemical Charge Transfer in the Hopping Regime**  
Xing Yin, Emil Wierzbinski, Hao Lu, Silvia Bezer, Arnie R. de Leon, Kathryn L. Davis, Catalina Achim,\* and David H. Waldeck\*
- 7590 dx.doi.org/10.1021/jp504139j  
**Microhydration of Contact Ion Pairs in  $\text{M}^{2+}\text{OH}^-(\text{H}_2\text{O})_{n=1-5}$  ( $\text{M} = \text{Mg, Ca}$ ) Clusters: Spectral Manifestations of a Mobile Proton Defect in the First Hydration Shell**  
Christopher J. Johnson, Laura C. Dzugan, Arron B. Wolk, Christopher M. Leavitt, Joseph A. Fournier, Anne B. McCoy,\* and Mark A. Johnson\*
- 7598 dx.doi.org/10.1021/jp5051657  
**S/G-1: An ab Initio Force-Field Blending Frozen Hermite Gaussian Densities and Distributed Multipoles. Proof of Concept and First Applications to Metal Cations**  
Robin Chaudret, Nohad Gresh, Christophe Narth, Louis Lagardère, Thomas A. Darden, G. Andrés Cisneros,\* and Jean-Philip Piquemal\*

**Infrared Photodissociation Spectroscopy of Microhydrated Nitrate–Nitric Acid Clusters  $\text{NO}_3^- (\text{HNO}_3)_m (\text{H}_2\text{O})_n$**   
Nadja Heine, Tara I. Yacovitch, Franziska Schubert, Claudia Briege, Daniel M. Neumark,\* and Knut R. Asmis\*