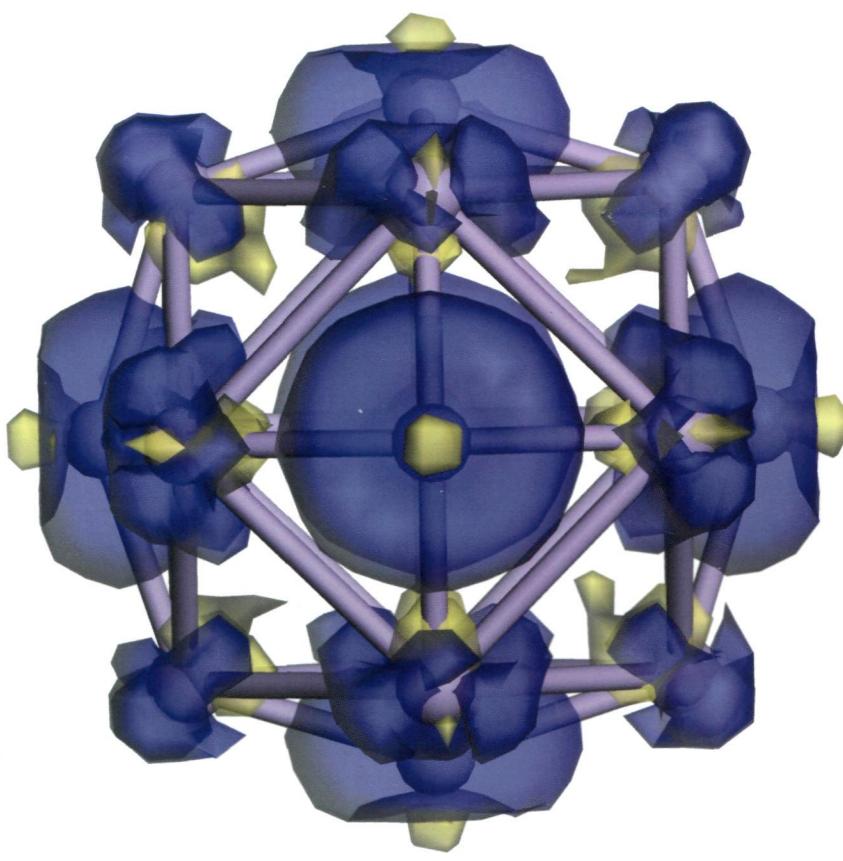


7M  
J 80/cp  
23 July 2013

Volume 139 Number 4

# AIP | The Journal of Chemical Physics



80<sup>th</sup>  
Anniversary

jcp.aip.org

► Cover image from Menghao Wu and Puru Jena, *J. Chem. Phys.* **138**, 044301 (2013).

## COMMUNICATIONS

**Communication: Some critical features of the potential energy surface for the  $\text{Cl} + \text{H}_2\text{O} \rightarrow \text{HCl} + \text{OH}$  forward and reverse reactions (4 pages)**

Yundong Guo, Meiling Zhang, Yaoming Xie, and Henry F. Schaefer III ..... 041101

**Communication: Fundamental equation of state correlation with hybrid data sets (4 pages)**

G. Rutkai, M. Thol, R. Lustig, R. Span, and J. Vrabec ..... 041102

**Communication: Long-range angular correlations in liquid water (4 pages)**

Yu Liu and Jianzhong Wu ..... 041103

## ARTICLES

### Theoretical Methods and Algorithms

**The multi-configuration self-consistent field method within a polarizable embedded framework (12 pages)**

Erik Donovan Hedegård, Nanna H. List, Hans Jørgen Aagaard Jensen, and Jacob Kongsted ..... 044101

**Higher-order kinetic expansion of quantum dissipative dynamics: Mapping quantum networks to kinetic networks (13 pages)**

Jianlan Wu and Jianshu Cao ..... 044102

**Qualitative change of character of dispersive interaction with intermolecular distance (5 pages)**

Johannes Haslmayr and Thomas Renger ..... 044103

**A novel Gaussian Binning (1GB) analysis of vibrational state distributions in highly excited  $\text{H}_2\text{O}$  from reactive quenching of  $\text{OH}^*$  by  $\text{H}_2$  (9 pages)**

Riccardo Conte, Bina Fu, Eugene Kamarchik, and Joel M. Bowman ..... 044104

**Adaptive single replica multiple state transition interface sampling (11 pages)**

Wei-Na Du and Peter G. Bolhuis ..... 044105

**Generalized coupling parameter expansion: Application to square well and Lennard-Jones fluids (7 pages)**

A. Sai Venkata Ramana ..... 044106

**Numerical integration of the extended variable generalized Langevin equation with a positive Prony representable memory kernel (11 pages)**

Andrew D. Baczewski and Stephen D. Bond ..... 044107

**Molecular dynamics study of the pressure-dependent terahertz infrared absorption spectrum of  $\alpha$ - and  $\gamma$ -RDX (7 pages)**

Andrey Pereverzov, Thomas D. Sewell, and Donald L. Thompson ..... 044108

**Development of a ReaxFF potential for Pd/O and application to palladium oxide formation (15 pages)**

Thomas P. Sengl, Randall J. Meyer, Michael J. Janik, and Adri C. T. van Duin ..... 044109

**Coupled electron-nuclear dynamics: Charge migration and charge transfer initiated near a conical intersection (12 pages)**

David Mendive-Tapia, Morgane Vacher, Michael J. Bearpark, and Michael A. Robb ..... 044110

<b>Vibrational solvatochromism: Towards systematic approach to modeling solvation phenomena (13 pages)</b>	
Bartosz Błasiak, Hochan Lee, and Minhaeng Cho . . . . .	044111
<b>Efficient antisymmetrization algorithm for the partially correlated wave functions in the free complement-local Schrödinger equation method (16 pages)</b>	
Hiroyuki Nakashima and Hiroshi Nakatsuji . . . . .	044112
<b>Energy and shape relaxation in binary atomic systems with realistic quantum cross sections (14 pages)</b>	
Reinel Sospedra-Alfonso and Bernie D. Shizgal . . . . .	044113
<b>General coalescence conditions for the exact wave functions: Higher-order relations for two-particle systems (7 pages)</b>	
Yusaku I. Kurokawa, Hiroyuki Nakashima, and Hiroshi Nakatsuji . . . . .	044114
<b>Entanglement dynamics of two qubits coupled individually to Ohmic baths (7 pages)</b>	
Liwei Duan, Hui Wang, Qing-Hu Chen, and Yang Zhao . . . . .	044115
<b>A comparison between state-specific and linear-response formalisms for the calculation of vertical electronic transition energy in solution with the CCSD-PCM method (9 pages)</b>	
Marco Caricato . . . . .	044116
<b>Influence of neighboring reactive particles on diffusion-limited reactions (10 pages)</b>	
Changsun Eun, Peter M. Kekenes-Huskey, and J. Andrew McCammon . . . . .	044117
<b>Multireference configuration interaction theory using cumulant reconstruction with internal contraction of density matrix renormalization group wave function (15 pages)</b>	
Masaaki Saitow, Yuki Kurashige, and Takeshi Yanai . . . . .	044118
<b>Comparison of volume and surface area nonpolar solvation free energy terms for implicit solvent simulations (6 pages)</b>	
Michael S. Lee and Mark A. Olson . . . . .	044119
<b>Boundary based on exchange symmetry theory for multilevel simulations. I. Basic theory (8 pages)</b>	
Motoyuki Shiga and Marco Masia . . . . .	044120

### Atoms, Molecules, and Clusters

<b>Magnetic hollow cages with colossal moments (6 pages)</b>	
Menghao Wu and Puru Jena . . . . .	044301
<b>Finite size line broadening and superradiance of optical transitions in two dimensional long-range ordered molecular aggregates (9 pages)</b>	
Mathias Müller, Alexander Paulheim, Alexander Eisfeld, and Moritz Sokolowski . . . . .	044302
<b>On the electronic structure of the low lying electronic states of vanadium trioxide (8 pages)</b>	
Elizabeth M. Y. Lee, Xiaolei Zhu, and David R. Yarkony . . . . .	044303
<b>Dissipative electron transfer dynamics in mixed valence dimers: Microscopic approach to the solid state problem (13 pages)</b>	
Andrew Palii, Cristian Bosch-Serrano, Juan Modesto Clemente-Juan, Eugenio Coronado, and Boris Tsukerblat . . . . .	044304
<b>Field-free orientation by a single-cycle THz pulse: The NaI and IBr molecules (8 pages)</b>	
Ze-Yu Zhao, Yong-Chang Han, Yin Huang, and Shu-Lin Cong . . . . .	044305
<b>Accurate theoretical study on 18 <math>\Lambda</math>-S and 50 <math>\Omega</math> states of CS in the gas phase: Potential energy curves, spectroscopic parameters, and spin-orbit coupling (15 pages)</b>	
Deheng Shi, Xianghong Niu, Jinfeng Sun, and Zunlue Zhu . . . . .	044306
<b>Laser initiated reactions in N<sub>2</sub>O clusters studied by time-sliced ion velocity imaging technique (9 pages)</b>	
Kenji Honma . . . . .	044307

<b>Photoelectron spectroscopy of boron-gold alloy clusters and boron boronyl clusters: <math>B_3Au_n^-</math> and <math>B_3(BO)_n^-</math> (<math>n = 1, 2</math>) (9 pages)</b>	Qiang Chen, Hui Bai, Hua-Jin Zhai, Si-Dian Li, and Lai-Sheng Wang . . . . .	044308
<b>Global <i>ab initio</i> ground-state potential energy surface of <math>N_4</math> (8 pages)</b>	Yuliya Paukku, Ke R. Yang, Zoltan Varga, and Donald G. Truhlar . . . . .	044309
<b>Structures, energies, and bonding in the water heptamer (9 pages)</b>	Nancy Acelas, Gina Hincapié, Doris Guerra, Jorge David, and Albeiro Restrepo . . . . .	044310
<b>The role of Rydberg states in photoionization of <math>NO_2</math> and <math>(NO^+, O^-)</math> ion pair formation induced by one VUV photon (12 pages)</b>	S. Marggi Poullain, K. Veyrinas, P. Billaud, M. Lebech, Y. J. Picard, R. R. Lucchese, and D. Dowek . . . . .	044311
<b>Photoelectron spectroscopy and theoretical study of <math>M(IO_3)_2^-</math> (<math>M = H, Li, Na, K</math>): Structural evolution, optical isomers, and hyperhalogen behavior (7 pages)</b>	Gao-Lei Hou, Miao Miao Wu, Hui Wen, Qiang Sun, Xue-Bin Wang, and Wei-Jun Zheng . . . . .	044312
<b>Jet spectroscopy of buckybowl: Electronic and vibrational structures in the <math>S_0</math> and <math>S_1</math> states of triphenylene and sumanene (8 pages)</b>	Sachi Kunishige, Megumi Kawabata, Masaaki Baba, Takaya Yamanaka, Yuki Morita, Shuhei Higashibayashi, and Hidehiro Sakurai . . . . .	044313

### Liquids, Glasses, and Crystals

<b>Observation of nanophase segregation in LiCl aqueous solutions from transient grating experiments (11 pages)</b>	L. E. Bove, C. Dreyfus, R. Torre, and R. M. Pick . . . . .	044501
<b>Path integral Monte Carlo study of quantum-hard sphere solids (13 pages)</b>	Luis M. Sesé . . . . .	044502
<b>Ultrafast dynamics of liquid water: Frequency fluctuations of the OH stretch and the HOH bend (7 pages)</b>	Sho Imoto, Sotiris S. Xantheas, and Shinji Saito . . . . .	044503
<b>Length scales and interfacial potentials in ion hydration (10 pages)</b>	Yu Shi and Thomas L. Beck . . . . .	044504
<b>Influence of Förster-type energy transfer on the vibrational relaxation of anionic hydration shells (8 pages)</b>	Stephan Lotze and Huib J. Bakker . . . . .	044505
<b>How a solute-pump/solvent-probe spectroscopy can reveal structural dynamics: Polarizability response spectra as a two-dimensional solvation spectroscopy (12 pages)</b>	Xiang Sun and Richard M. Stratt . . . . .	044506
<b>Structure and properties of sodium aluminosilicate glasses from molecular dynamics simulations (17 pages)</b>	Ye Xiang, Jincheng Du, Morten M. Smedskjaer, and John C. Mauro . . . . .	044507
<b>The influence of trehalose on hydrophobic interactions of small nonpolar solute: A molecular dynamics simulation study (9 pages)</b>	Subrata Paul and Sandip Paul . . . . .	044508
<b>Cooperative dynamic and diffusion behavior above and below the dynamical crossover of supercooled water (7 pages)</b>	Germán C. Picasso, David C. Malaspina, Marcelo A. Carignano, and Igal Szleifer . . . . .	044509
<b>Linear and nonlinear density response functions for a simple atomic fluid (12 pages)</b>	Benjamin A. Dalton, Kirill S. Glavatskiy, Peter J. Daivis, B. D. Todd, and Ian K. Snook . . . . .	044510

## Surfaces, Interfaces, and Materials

<b>Scale effects in the latent heat of melting in nanopores (4 pages)</b>		
J.-H. Shin, J.-Y. Parlange, and M. R. Deinert .....		044701
<b>Ferroelectric mechanism of croconic acid: A first-principles and Monte Carlo study (6 pages)</b>		
Yaxuan Cai, Shijun Luo, Zhanwu Zhu, and Haoshuang Gu .....		044702
<b>Charge-induced distortion and stabilization of surface transfer doped porphyrin films (6 pages)</b>		
Y. Smets, C. B. Stark, S. Lach, F. Schmitt, C. A. Wright, M. Wanke, L. Ley, C. Ziegler, and C. I. Pakes .....		044703
<b>On the Green-Kubo relationship for the liquid-solid friction coefficient (4 pages)</b>		
Lydéric Bocquet and Jean-Louis Barrat .....		044704
<b>Methanol synthesis on ZnO(000̄1). II. Structure, energetics, and vibrational signature of reaction intermediates (17 pages)</b>		
Janos Kiss, Johannes Frenzel, Bernd Meyer, and Dominik Marx .....		044705
<b>Diffusion, adsorption, and desorption of molecular hydrogen on graphene and in graphite (12 pages)</b>		
Justin Petucci, Carl LeBlond, Majid Karimi, and Gianfranco Vidali .....		044706
<b>On the fly first principles study of the classical scattering of an Ar atom from the LiF(100) surface (8 pages)</b>		
Asaf Azuri and Eli Pollak .....		044707
<b>Comparative study of phenol and thiophenol adsorption on Cu(110) (6 pages)</b>		
Y. Kitaguchi, S. Habuka, T. Mitsui, H. Okuyama, S. Hatta, and T. Aruga .....		044708
<b>Origin of anomalous strain effects on the molecular adsorption on boron-doped graphene (7 pages)</b>		
Joongoo Kang, Yong-Hyun Kim, Greg C. Glatzmaier, and Su-Huai Wei .....		044709
<b>First-principles thermodynamic screening approach to photo-catalytic water splitting with co-catalysts (5 pages)</b>		
Harald Oberhofer and Karsten Reuter .....		044710
<b>Chirality dependence of quantum thermal transport in carbon nanotubes at low temperatures: A first-principles study (8 pages)</b>		
Tomoyuki Hata, Hiroki Kawai, Tatsuhiko Ohto, and Koichi Yamashita .....		044711
<b>Adsorption of hydrogen on the surface and sub-surface of Cu(111) (8 pages)</b>		
Kumudu Mudiyanselage, Yixiong Yang, Friedrich M. Hoffmann, Octavio J. Furlong, Jan Hrbek, Michael G. White, Ping Liu, and Darío J. Stacchiola .....		044712
<b>Hollow gold nanorectangles: The roles of polarization and substrate (7 pages)</b>		
Rachel D. Near and Mostafa A. El-Sayed .....		044713
<b>First principles study of hydroxyapatite surface (8 pages)</b>		
Alexander Slepko and Alexander A. Demkov .....		044714
<b>Surface-enhanced Raman spectroscopic studies of the Au-pentacene interface: A combined experimental and theoretical investigation (8 pages)</b>		
D. Adil and S. Guha .....		044715
<b>Proton dynamics in ice VII at high pressures (9 pages)</b>		
Y. Finkelstein and R. Moreh .....		044716

## Polymers and Soft Matter

<b>Shape characteristics of equilibrium and non-equilibrium fractal clusters (11 pages)</b>		
Marc L. Mansfield and Jack F. Douglas .....		044901

<b>Polymer translocation through a gradient channel (6 pages)</b>		
Shuang Zhang, Chao Wang, Li-Zhen Sun, Chao-Yang Li, and Meng-Bo Luo . . . . .	044902	
<b>Resonance Raman overtones reveal vibrational displacements and dynamics of crystalline and amorphous poly(3-hexylthiophene) chains in fullerene blends (9 pages)</b>		
Jian Gao and John K. Grey . . . . .	044903	
<b>Effects of the dipolar interaction on the equilibrium morphologies of a single supramolecular magnetic filament in bulk (9 pages)</b>		
Pedro A. Sánchez, Joan J. Cerdà, Tomás Sintes, and Christian Holm . . . . .	044904	
<b>Modified scaling principle for rotational relaxation in a model for suspensions of rigid rods (18 pages)</b>		
Ying-Lung Steve Tse and Hans C. Andersen . . . . .	044905	
<b>Modeling the collective relaxation time of glass-forming polymers at intermediate length scales: Application to polyisobutylene (6 pages)</b>		
Juan Colmenero, Fernando Alvarez, Yasmin Khairy, and Arantxa Arbe . . . . .	044906	
<b>Alteration of gas phase ion polarizabilities upon hydration in high dielectric liquids (11 pages)</b>		
Sahin Buyukdagli and T. Ala-Nissila . . . . .	044907	
<b>Kinetics of particle wrapping by a vesicle (11 pages)</b>		
Stephen Mirigian and Murugappan Muthukumar . . . . .	044908	
<b>Second-order resummed thermodynamic perturbation theory for central-force associating potential: Multi-patch colloidal models (9 pages)</b>		
Y. V. Kalyuzhnyi, B. D. Marshall, W. G. Chapman, and P. T. Cummings . . . . .	044909	
<b>Conformational switching of modified guest chains in polymer brushes (11 pages)</b>		
D. Romeis and J.-U. Sommer . . . . .	044910	
<b>Effects of domain morphology on kinetics of fluid phase separation (10 pages)</b>		
Sutapa Roy and Subir K. Das . . . . .	044911	
<b>Confinement dynamics of a semiflexible chain inside nano-spheres (8 pages)</b>		
A. Fathizadeh, Maziar Heidari, B. Eslami-Mossallam, and M. R. Ejtehadi . . . . .	044912	
<b>Dendritic brushes under theta and poor solvent conditions (10 pages)</b>		
Leonidas N. Gergidis, Andreas Kalogirou, Antonios Charalambopoulos, and Costas Vlahos . . . . .	044913	

### Biological Molecules and Networks

<b>Low absorption state of phycocyanin from <i>Acaryochloris marina</i> antenna system: On the interplay between ionic strength and excitonic coupling (9 pages)</b>		
Collins Nganou . . . . .	045101	
<b>Proteins in the electric field near the surface of mica (9 pages)</b>		
Anna Starzyk and Marek Cieplak . . . . .	045102	
<b>Effect of quantum tunneling on single strand breaks in a modeled gas phase cytidine nucleotide induced by low energy electron: A theoretical approach (9 pages)</b>		
Renjith Bhaskaran and Manabendra Sarma . . . . .	045103	
<b>Critical fluctuations in DOPC/DPPC-d<sub>62</sub>/cholesterol mixtures: <sup>2</sup>H magnetic resonance and relaxation (10 pages)</b>		
James H. Davis, Latifa Ziani, and Miranda L. Schmidt . . . . .	045104	
<b>Scaling analysis of bio-molecular dynamics derived from elastic incoherent neutron scattering experiments (16 pages)</b>		
W. Doster, H. Nakagawa, and M. S. Appavou . . . . .	045105	

**LETTERS TO THE EDITOR****Notes**

- Note: The universal relations for the critical point parameters (2 pages)**  
E. M. Apfelbaum and V. S. Vorob'ev ..... 046101
- Note: Is it symmetric or not? (3 pages)**  
John F. Stanton ..... 046102

**Comments**

- Comment on "Experimental evidence for excess entropy discontinuities in glass-forming solutions"**  
[J. Chem. Phys. 136, 074515 (2012)] (2 pages)  
Anatoli Bogdan and Thomas Loerting ..... 047101
- Response to "Comment on 'Experimental evidence for excess entropy discontinuities in glass-forming solutions'" [J. Chem. Phys. 139, 047101 (2013)] (2 pages)**  
Daniel M. Lienhard, Bernhard Zobrist, Andreas Zuernd, Ulrich K. Krieger, and Thomas Peter ..... 047102

**Errata**

- Publisher's Note: "Monte Carlo and theoretical calculations of the first four perturbation coefficients in the high temperature series expansion of the free energy for discrete and core-softened potential models" [J. Chem. Phys. 138, 244115 (2013)] (1 page)**  
Shiqi Zhou and J. R. Solana ..... 049901
- Erratum: "First principle evaluation of the chiroptical activity of the di-phenyl-diazene derivatives"**  
[J. Chem. Phys. 137, 124307 (2012)] (1 page)  
Enrico Benassi and Stefano Corni ..... 049902