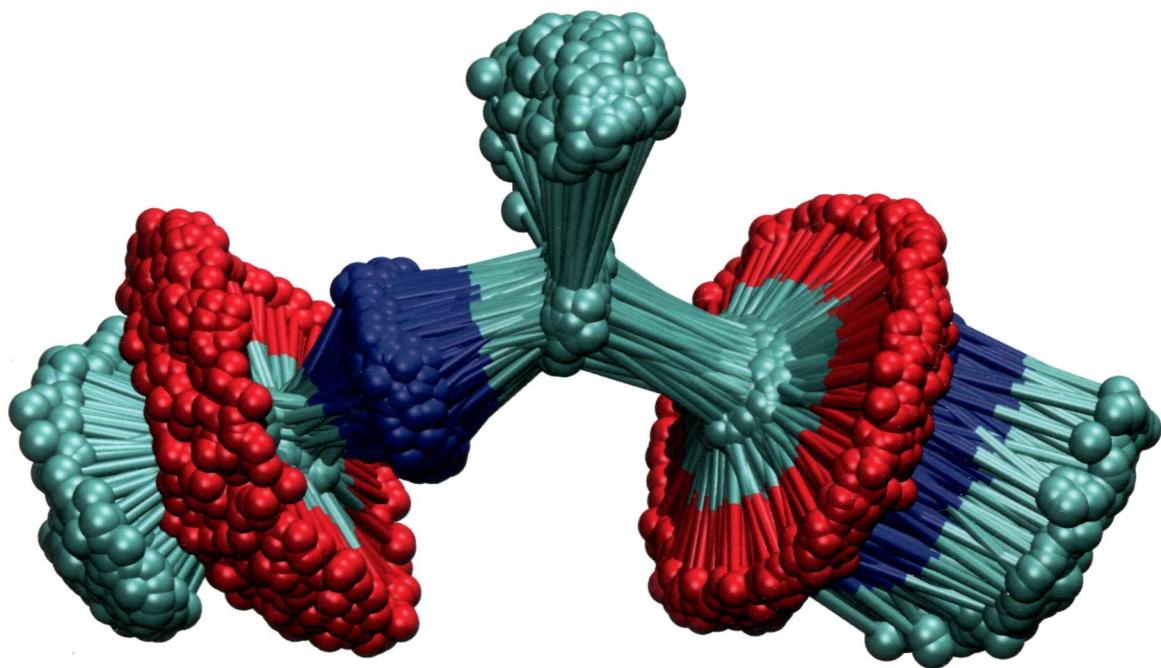


7 December 2013

Volume 139 Number 21

7/11  
J80/cp

# AIP | The Journal of Chemical Physics



80<sup>th</sup>  
Anniversary

jcp.aip.org

► Cover image from Behrooz Hashemian, Daniel Millán, and Marino Arroyo, *J. Chem. Phys.* **139**, 214101 (2013).

## COMMUNICATIONS

**Communication: The correct interpretation of surface hopping trajectories: How to calculate electronic properties (4 pages)**

Brian R. Landry, Martin J. Falk, and Joseph E. Subotnik ..... 211101

**Communication: A reduced-space algorithm for the solution of the complex linear response equations used in coupled cluster damped response theory (4 pages)**

Joanna Kauczor, Patrick Norman, Ove Christiansen, and Sonia Coriani ..... 211102

## ARTICLES

### Theoretical Methods and Algorithms

**Modeling and enhanced sampling of molecular systems with smooth and nonlinear data-driven collective variables (12 pages)**

Behrooz Hashemian, Daniel Millán, and Marino Arroyo ..... 214101

**Extended Lagrangian Born-Oppenheimer molecular dynamics in the limit of vanishing self-consistent field optimization (6 pages)**

Petros Souvatzis and Anders M. N. Niklasson ..... 214102

**Linear-scaling calculation of Hartree-Fock exchange energy with non-orthogonal generalised Wannier functions (16 pages)**

J. Dziedzic, Q. Hill, and C.-K. Skylaris ..... 214103

**An improved fragment-based quantum mechanical method for calculation of electrostatic solvation energy of proteins (13 pages)**

Xiangyu Jia, Xianwei Wang, Jinfeng Liu, John Z. H. Zhang, Ye Mei, and Xiao He ..... 214104

**Hamilton-Jacobi method for molecular distribution function in a chemical oscillator (11 pages)**

Hiizu Nakanishi, Takahiro Sakaue, and Jun'ichi Wakou ..... 214105

**Resummed thermodynamic perturbation theory for bond cooperativity in associating fluids (6 pages)**

Bennett D. Marshall and Walter G. Chapman ..... 214106

**Can we derive Tully's surface-hopping algorithm from the semiclassical quantum Liouville equation?**

**Almost, but only with decoherence (16 pages)**

Joseph E. Subotnik, Wenjun Ouyang, and Brian R. Landry ..... 214107

**Time dependent quantum thermodynamics of a coupled quantum oscillator system in a small thermal environment (10 pages)**

George L. Barnes and Michael E. Kellman ..... 214108

**Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory (9 pages)**

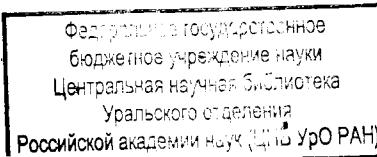
Erin R. Johnson, Alberto Otero-de-la-Roza, Stephen G. Dale, and Gino A. DiLabio ..... 214109

**Self-consistent continuum solvation (SCCS): The case of charged systems (8 pages)**

C. Dupont, O. Andreussi, and N. Marzari ..... 214110

(Continued)

A1



© 2013 AIP Publishing LLC

<b>Proximal distributions from angular correlations: A measure of the onset of coarse-graining (11 pages)</b>	
Kippi M. Dyer and B. Montgomery Pettitt .....	214111
<b>A minimally-resolved immersed boundary model for reaction-diffusion problems (15 pages)</b>	
Amneet Pal Singh Bhalla, Boyce E. Griffith, Neelesh A. Patankar, and Aleksandar Donev .....	214112
<b>The Stokes-Einstein relation at moderate Schmidt number (11 pages)</b>	
Florencio Balboa Usabiaga, Xiaoyi Xie, Rafael Delgado-Buscalioni, and Aleksandar Donev .....	214113
<b>Spin-free Dirac-Coulomb calculations augmented with a perturbative treatment of spin-orbit effects at the Hartree-Fock level (11 pages)</b>	
Lan Cheng, Stella Stopkowicz, and Jürgen Gauss .....	214114
<b>Diffusion in narrow channels on curved manifolds (7 pages)</b>	
Guillermo Chacón-Acosta, Inti Pineda, and Leonardo Dagdug .....	214115

### Advanced Experimental Techniques

<b>Observation of strongly forbidden solid effect dynamic nuclear polarization transitions via electron-electron double resonance detected NMR (6 pages)</b>	
Albert A. Smith, Björn Corzilius, Olesya Haze, Timothy M. Swager, and Robert G. Griffin .....	214201

### Atoms, Molecules, and Clusters

<b>Shape resonances in low-energy-electron collisions with halopyrimidines (7 pages)</b>	
Alessandra Souza Barbosa and Márcio H. F. Bettega .....	214301
<b>Simulation of femtosecond “double-slit” experiments for a chromophore in a dissipative environment (12 pages)</b>	
M. F. Gelin, Y. Tanimura, and W. Domcke .....	214302
<b>Thermal decomposition products of butyraldehyde (9 pages)</b>	
Courtney D. Hatten, Kevin R. Kaskey, Brian J. Warner, Emily M. Wright, and Laura R. McCunn .....	214303
<b>Solvent effects on the ultrafast nonradiative deactivation mechanisms of thymine in aqueous solution: Excited-state QM/MM molecular dynamics simulations (11 pages)</b>	
Akira Nakayama, Gaku Arai, Shohei Yamazaki, and Tetsuya Taketsugu .....	214304
<b>Theoretical study of <math>\text{Al}_n\text{V}^+</math> clusters and their interaction with Ar (8 pages)</b>	
Eva María Fernández, Andrés Vega, and Luis Carlos Balbás .....	214305
<b>Non-Markovian response of ultrafast coherent electronic ring currents in chiral aromatic molecules in a condensed phase (8 pages)</b>	
H. Mineo, S. H. Lin, Y. Fujimura, J. Xu, R. X. Xu, and Y. J. Yan .....	214306
<b>Trends in alkali metal hydrosulfides: A combined Fourier transform microwave/millimeter-wave spectroscopic study of KSH (<math>\tilde{\chi}^1\text{A}'</math>) (10 pages)</b>	
M. P. Buccino, P. M. Sheridan, J. P. Young, M. K. L. Binns, D. W. Ewing, and L. M. Ziurys .....	214307
<b>Energy and charge transfer in ionized argon coated water clusters (7 pages)</b>	
J. Kočíšek, J. Lengyel, M. Fárník, and P. Slavíček .....	214308
<b>Infrared spectra and tunneling dynamics of the <math>\text{N}_2\text{-D}_2\text{O}</math> and <math>\text{OC-D}_2\text{O}</math> complexes in the <math>\nu_2</math> bend region of <math>\text{D}_2\text{O}</math> (6 pages)</b>	
Yu Zhu, Rui Zheng, Song Li, Yu Yang, and Chuanxi Duan .....	214309
<b>A new look at the photodissociation of methyl iodide at 193 nm (8 pages)</b>	
Hong Xu and S. T. Pratt .....	214310

**Lowest triplet ( $n, \pi^*$ ) state of 2-cyclohexen-1-one: Characterization by cavity ringdown spectroscopy and quantum-chemical calculations (12 pages)**

- Michael O. McAnally, Katherine L. Zabronsky, Daniel J. Stupca, Kaitlyn Phillipson,  
Nathan R. Pillsbury, and Stephen Drucker ..... 214311

**Liquids, Glasses, and Crystals****NMR  $T_1$  relaxation time measurements and calculations with translational and rotational components for liquid electrolytes containing LiBF<sub>4</sub> and propylene carbonate (11 pages)**

- P. M. Richardson, A. M. Voice, and I. M. Ward ..... 214501

**The dynamical crossover in attractive colloidal systems (12 pages)**

- Francesco Mallamace, Carmelo Corsaro, H. Eugene Stanley, Domenico Mallamace,  
and Sow-Hsin Chen ..... 214502

**Phase diagram of ammonium nitrate (11 pages)**

- Mihindra Dunuwille and Choong-Shik Yoo ..... 214503

**Surfaces, Interfaces, and Materials****The liquid surface of chiral ionic liquids as seen from molecular dynamics simulations combined with intrinsic analysis (15 pages)**

- Martin Lísal ..... 214701

***In situ* self-assembled organic interface layers for the controlled growth of oligothiophene thin films on ferroelectric Pb(Zr<sub>0.2</sub>Ti<sub>0.8</sub>)O<sub>3</sub> (7 pages)**

- P. Milde, R. Schönenfelder, A. Koitzsch, K. Haubner, U. Zerweck-Trogisch, E. Jaehne,  
and L. M. Eng ..... 214702

**Vapor condensation onto a non-volatile liquid drop (10 pages)**

- Levent Inci and Richard K. Bowles ..... 214703

**A fragment method for systematic improvement of anharmonic adsorbate vibrational frequencies: Acetylene on Cu(001) (8 pages)**

- Sergey K. Chulkov and David M. Benoit ..... 214704

**Phase stabilities at a glance: Stability diagrams of nickel dipnictides (9 pages)**

- F. Bachhuber, J. Rothbäller, T. Söhnle, and R. Weihrich ..... 214705

**Barrier height formation in organic blends/metal interfaces: Case of tetrathiafulvalene-tetracyanoquinodimethane/Au(111) (8 pages)**

- José I. Martínez, Enrique Abad, Juan I. Beltrán, Fernando Flores, and José Ortega ..... 214706

**Methane dissociative chemisorption and detailed balance on Pt(111): Dynamical constraints and the modest influence of tunneling (15 pages)**

- S. B. Donald, J. K. Navin, and I. Harrison ..... 214707

**Vibration responses of *h*-BN sheet to charge doping and external strain (6 pages)**

- Wei Yang, Yu Yang, Fawei Zheng, and Ping Zhang ..... 214708

**Manipulating transport through a single-molecule junction (5 pages)**

- Kai Sotthewes, René Heimbuch, and Harold J. W. Zandvliet ..... 214709

**Electronic excitations of bulk LiCl from many-body perturbation theory (5 pages)**

- Yun-Feng Jiang, Neng-Ping Wang, and Michael Rohlfing ..... 214710

**Polymers and Soft Matter****Microstructure and magnetic properties of magnetic fluids consisting of shifted dipole particles under the influence of an external magnetic field (12 pages)**

- Rudolf Weeber, Marco Klinkigt, Sofia Kantorovich, and Christian Holm ..... 214901

(Continued)

<b>Binary mixed homopolymer brushes grafted on nanorod particles: A self-consistent field theory study (10 pages)</b>	
Xin Ma, Yingzi Yang, Lei Zhu, Bin Zhao, Ping Tang, and Feng Qiu .....	214902
<b>Conformation and elasticity of a charged polymer chain bridging two nanoparticles (11 pages)</b>	
W. Nowicki and G. Nowicka .....	214903
<b>Crystallization mechanism in melts of short n-alkane chains (5 pages)</b>	
Muhammad Anwar, Francesco Turci, and Tanja Schilling .....	214904
<b>Fluctuation effects on the order-disorder transition in polydisperse copolymer melts (12 pages)</b>	
Gunja Pandav and Venkat Ganesan .....	214905

### Biological Molecules and Networks

<b>Spatio-temporal hierarchy in the dynamics of a minimalist protein model (13 pages)</b>	
Yasuhiro Matsunaga, Akinori Baba, Chun-Biu Li, John E. Straub, Mikito Toda, Tamiki Komatsuzaki, and R. Stephen Berry .....	215101
<b>Slow dynamics of a protein backbone in molecular dynamics simulation revealed by time-structure based independent component analysis (10 pages)</b>	
Yusuke Naritomi and Sotaro Fuchigami .....	215102

### LETTERS TO THE EDITOR

#### Comments

<b>Comment on “Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. I. Statics” [J. Chem. Phys. 134, 204904 (2011)] (2 pages)</b>	
J. P. Wittmer, H. Meyer, A. Johner, S. Obukhov, and J. Baschnagel .....	217101
<b>Response to “Comment on ‘Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. I. Statics’” [J. Chem. Phys. 139, 217101 (2013)] (2 pages)</b>	
Jonathan D. Halverson, Won Bo Lee, Gary S. Grest, Alexander Y. Grosberg, and Kurt Kremer .....	217102