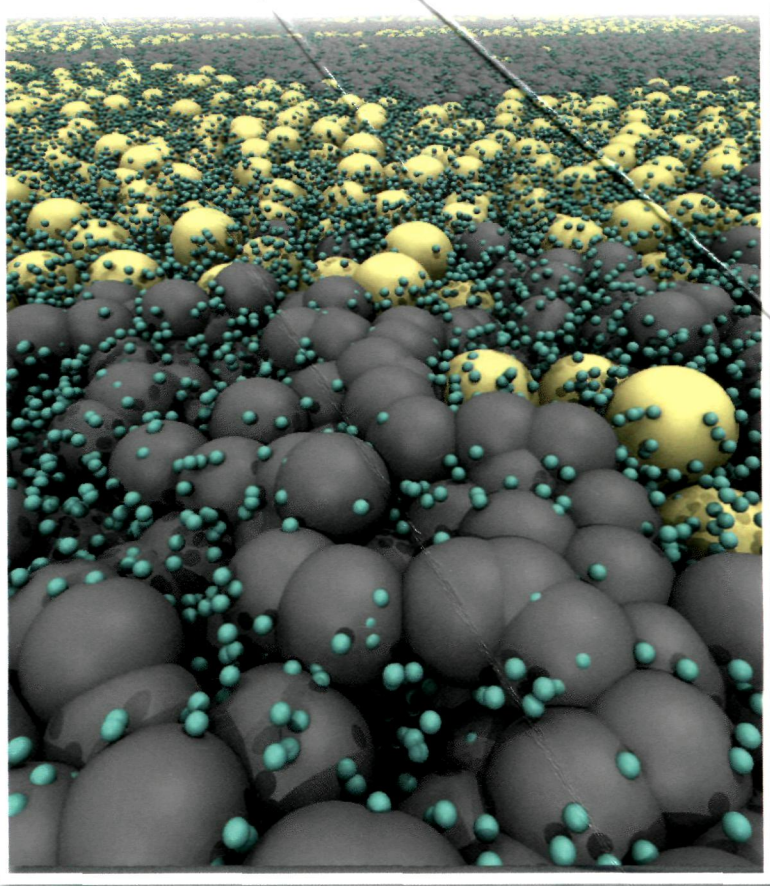


ПН  
780/CP  
MAY 2013

Volume 138 Number 5

# AIP | The Journal of Chemical Physics



80<sup>th</sup>  
Anniversary

[jcp.aip.org](http://jcp.aip.org)

► **Cover image** from Alexander Winkler, Peter Virnau, Kurt Binder, Roland G. Winkler, and Gerhard Gompper, *J. Chem. Phys.* **138**, 054901 (2013).

## COMMUNICATIONS

- Communication: Transfer of more than half the population to a selected rovibrational state of H<sub>2</sub> by Stark-induced adiabatic Raman passage (4 pages)**  
Nandini Mukherjee, Wenrui Dong, John A. Harrison, and Richard N. Zare ..... 051101
- Communication: Biexciton generation rates in CdSe nanorods are length independent (4 pages)**  
Roi Baer and Eran Rabani ..... 051102

## ARTICLES

### Theoretical Methods and Algorithms

- An accurate and linear-scaling method for calculating charge-transfer excitation energies and diabatic couplings (12 pages)**  
Michele Pavanello, Troy Van Voorhis, Lucas Visscher, and Johannes Neugebauer ..... 054101
- Coupling of kinetic Monte Carlo simulations of surface reactions to transport in a fluid for heterogeneous catalytic reactor modeling (9 pages)**  
C. Schaefer and A. P. J. Jansen ..... 054102
- Many-body dispersion interactions from the exchange-hole dipole moment model (10 pages)**  
A. Otero-de-la-Roza and Erin R. Johnson ..... 054103
- Signatures of discrete breathers in coherent state quantum dynamics (11 pages)**  
Kirill Igumenshchev, Misha Ovchinnikov, Panagiotis Maniadis, and Oleg Prezhdo ..... 054104
- A quadratically convergent VBSCF method (9 pages)**  
Zahid Rashid and Joop H. van Lenthe ..... 054105
- Reaction coordinates, one-dimensional Smoluchowski equations, and a test for dynamical self-consistency (13 pages)**  
Baron Peters, Peter G. Bolhuis, Ryan G. Mullen, and Joan-Emma Shea ..... 054106
- The Schrödinger equation with friction from the quantum trajectory perspective (7 pages)**  
Sophya Garashchuk, Vaibhav Dixit, Bing Gu, and James Mazzuca ..... 054107
- Structural fluctuation of protein in water around its native state: A new statistical mechanics formulation (11 pages)**  
Bongsoo Kim and Fumio Hirata ..... 054108
- The orbital-specific virtual local triples correction: OSV-L(T) (10 pages)**  
Martin Schütz, Jun Yang, Garnet Kin-Lic Chan, Frederick R. Manby, and Hans-Joachim Werner ..... 054109
- Going beyond the frozen core approximation: Development of coordinate-dependent pseudopotentials and application to Na<sub>2</sub><sup>+</sup> (9 pages)**  
Argyris Kahros and Benjamin J. Schwartz ..... 054110

<b>Modeling molecular response in uniform and non-uniform electric fields</b> (9 pages)	
Michael Morris and Meredith J. T. Jordan	054111
<b>Generalized Born forces: Surface integral formulation</b> (11 pages)	
Federico Fogolari, Alessandra Corazza, and Gennaro Esposito	054112
<b>NMR chemical shift as analytical derivative of the Helmholtz free energy</b> (10 pages)	
Willem Van den Heuvel and Alessandro Soncini	054113
<b>Development of polaron-transformed explicitly correlated full configuration interaction method for investigation of quantum-confined Stark effect in GaAs quantum dots</b> (6 pages)	
Christopher J. Blanton, Christopher Brenon, and Arindam Chakraborty	054114
<b>A relative entropy rate method for path space sensitivity analysis of stationary complex stochastic dynamics</b> (16 pages)	
Yannis Pantazis and Markos A. Katsoulakis	054115
<b>Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme</b> (13 pages)	
Michele Ceotto, Yu Zhuang, and William L. Hase	054116
<b>Polarizability effects in molecular dynamics simulations of the graphene-water interface</b> (9 pages)	
Tuan A. Ho and Alberto Striolo	054117
<b>Quantum dynamical structure factor of liquid neon via a quasiclassical symmetrized method</b> (10 pages)	
Michele Monteferrante, Sara Bonella, and Giovanni Ciccotti	054118
<b>A variational formulation of electrostatics in a medium with spatially varying dielectric permittivity</b> (13 pages)	
Vikram Jadhao, Francisco J. Solis, and Monica Olvera de la Cruz	054119
<b>Combined-hyperbolic-inverse-power-representation of potential energy surfaces: A preliminary assessment for H<sub>3</sub> and HO<sub>2</sub></b> (14 pages)	
A. J. C. Varandas	054120

### Advanced Experimental Techniques

<b>New insights for accurate chemically specific measurements of slow diffusing molecules</b> (8 pages)	
Jianbo Hou and Louis A. Madsen	054201

### Atoms, Molecules, and Clusters

<b>Photodissociation dynamics of the methyl perthiyl radical at 248 nm via photofragment translational spectroscopy</b> (5 pages)	
Neil C. Cole-Filipiak, Bogdan Negru, Gabriel M. P. Just, Dayoung Park, and Daniel M. Neumark	054301
<b>A comprehensive and comparative study of elastic electron scattering from OCS and CS<sub>2</sub> in the energy region from 1.2 to 200 eV</b> (12 pages)	
H. Murai, Y. Ishijima, T. Mitsumura, Y. Sakamoto, H. Kato, M. Hoshino, F. Blanco, G. García, P. Limão-Vieira, M. J. Brunger, S. J. Buckman, and H. Tanaka	054302
<b>Bimetallic cages</b> (8 pages)	
René Fournier and Sabeen Afzal-Hussain	054303
<b>Fast excited state dynamics in the isolated 7-azaindole-phenol H-bonded complex</b> (9 pages)	
Marcela C. Capello, Michel Broquier, Claude Dedonder-Lardeux, Christophe Jouvét, and Gustavo A. Pino	054304

<b>Time-dependent wave packet state-to-state dynamics of H/D + HCl/DCI reactions (12 pages)</b> Hongwei Song, Soo-Y Lee, Zhigang Sun, and Yunpeng Lu .....	054305
<b>Ions interacting with planar aromatic molecules: Modeling electron transfer reactions (8 pages)</b> B. O. Forsberg, J. D. Alexander, T. Chen, A. T. Pettersson, M. Gatchell, H. Cederquist, and H. Zettergren .....	054306
<b>Reactions between atomic chlorine and pyridine in solid <i>para</i>-hydrogen: Infrared spectrum of the 1-chloropyridinyl (C<sub>5</sub>H<sub>5</sub>N–Cl) radical (10 pages)</b> Prasanta Das, Mohammed Bahou, and Yuan-Pern Lee .....	054307
<b>First principles exploration of NiO and its ions NiO<sup>+</sup> and NiO<sup>-</sup> (15 pages)</b> Constantine N. Sakellaris and Aristides Mavridis .....	054308
<b>Structure and properties of Mn<sub>4</sub>Cl<sub>9</sub>: An antiferromagnetic binary hyperhalogen (6 pages)</b> Yawei Li, Shunhong Zhang, Qian Wang, and Puru Jena .....	054309
<b>Role of zero-point vibrational corrections to carbon hyperfine coupling constants in organic <math>\pi</math> radicals (8 pages)</b> X. Chen, Z. Rinkevicius, K. Ruud, and H. Ågren .....	054310
<b>Photodetachment anisotropy for mixed <i>s-p</i> states: 8/3 and other fractions (14 pages)</b> Andrei Sanov, Emily R. Grumbling, Daniel J. Goebbert, and Lori M. Culbertson .....	054311
<b>Excitonic states in a (Ti<sub>6</sub>O<sub>12</sub>)<sub>3</sub> nanotube (6 pages)</b> B. N. Papas and J. L. Whitten .....	054312
<b>State-to-state three-atom time-dependent reactive scattering in hyperspherical coordinates (12 pages)</b> Jeff Crawford and Gregory A. Parker .....	054313
<b>The localization tensor for the H<sub>2</sub> molecule: Closed formulae for the Heitler-London and related wavefunctions and comparison with full configuration interaction (9 pages)</b> Celestino Angeli, Gian Luigi Bendazzoli, and Stefano Evangelisti .....	054314
<b>Liquids, Glasses, and Crystals</b>	
<b>Size and rate dependence of crystal nucleation in single tin drops by fast scanning calorimetry (5 pages)</b> Bin Yang, A. S. Abyzov, E. Zhuravlev, Yulai Gao, J. W. P. Schmelzer, and C. Schick .....	054501
<b>Orientation correlation of p-nitroaniline molecules in acetone solution observed by hyper-Rayleigh scattering (7 pages)</b> David P. Shelton .....	054502
<b>New form of polymeric nitrogen from dynamic shock simulation (8 pages)</b> Todd D. Beudet, William D. Mattson, and Betsy M. Rice .....	054503
<b>Effect of presence of salt on the dynamics of water in uncharged nanochannels (7 pages)</b> Chirodeep Bakli and Suman Chakraborty .....	054504
<b>Equation of state, refractive index and polarizability of compressed water to 7 GPa and 673 K (9 pages)</b> Carmen Sanchez-Valle, Davide Mantegazzi, Jay D. Bass, and Eric Reusser .....	054505
<b>Molecular origin of the difference in the HOH bend of the IR spectra between liquid water and ice (8 pages)</b> Sho Imoto, Sotiris S. Xantheas, and Shinji Saito .....	054506
<b>Liquid-vapor phase diagram and surface properties in oppositely charged colloids represented by a mixture of attractive and repulsive Yukawa potentials (18 pages)</b> Gustavo A. Chapela, Fernando del Río, and José Alejandre .....	054507
<b>Compressed correlation functions and fast aging dynamics in metallic glasses (6 pages)</b> B. Ruta, G. Baldi, G. Monaco, and Y. Chushkin .....	054508

### Surfaces, Interfaces, and Materials

- Diamond as an inert substrate of graphene** (4 pages)  
Wei Hu, Zhenyu Li, and Jinlong Yang ..... 054701
- An X-ray absorption spectroscopy study of the inversion degree in zinc ferrite nanocrystals dispersed on a highly porous silica aerogel matrix** (9 pages)  
D. Carta, C. Marras, D. Loche, G. Mountjoy, S. I. Ahmed, and A. Corrias ..... 054702
- Density functional study of the stability of various  $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> surfaces** (7 pages)  
Yan-Hua Lei and Zhao-Xu Chen ..... 054703
- Thermodynamic and kinetic theory of nucleation, deliquescence and efflorescence transitions in the ensemble of droplets on soluble particles** (12 pages)  
Alexander K. Shchekin, Ilya V. Shabaev, and Olaf Hellmuth ..... 054704
- Determination of the charge neutrality level of poly(3-hexylthiophene)** (9 pages)  
Wenfeng Wang, Jan H. Alsmeier, Matthäus Wolak, and Rudy Schlaf ..... 054705
- Theoretical studies of lithium incorporation into  $\alpha$ -Sn(100)** (4 pages)  
Payam Kaghazchi ..... 054706
- Shear behavior of a confined thin film: Influence of the molecular dynamics scheme employed** (11 pages)  
Hai Hoang and Guillaume Galliero ..... 054707
- Simulation study for adsorption-induced structural transition in stacked-layer porous coordination polymers: Equilibrium and hysteretic adsorption behaviors** (10 pages)  
Ryohei Numaguchi, Hideki Tanaka, Satoshi Watanabe, and Minoru T. Miyahara ..... 054708

### Polymers and Soft Matter

- Hydrodynamic mechanisms of spinodal decomposition in confined colloid-polymer mixtures: A multiparticle collision dynamics study** (14 pages)  
Alexander Winkler, Peter Virnau, Kurt Binder, Roland G. Winkler, and Gerhard Gompper ..... 054901
- Translocation dynamics of a short polymer driven by an oscillating force** (7 pages)  
Nicola Pizzolato, Alessandro Fiasconaro, Dominique Persano Adorno,  
and Bernardo Spagnolo ..... 054902
- Unified explanation of the anomalous dynamic properties of highly asymmetric polymer blends** (17 pages)  
K. L. Ngai and S. Capaccioli ..... 054903
- Gyration tensor based analysis of the shapes of polymer chains in an attractive spherical cage** (8 pages)  
Handan Arkin and Wolfhard Janke ..... 054904
- Minimal energy packings of nearly flexible polymers** (7 pages)  
Robert S. Hoy, Jared Harwayne-Gidansky, and Corey S. O'Hern ..... 054905
- The vibration properties of the (n,0) boron nitride nanotubes from *ab initio* quantum chemical simulations** (9 pages)  
A. Erba, M. Ferrabone, J. Baima, R. Orlando, M. Rérat, and R. Dovesi ..... 054906

### Biological Molecules and Networks

- Molecular noise induces concentration oscillations in chemical systems with stable node steady states** (18 pages)  
D. L. K. Toner and R. Grima ..... 055101