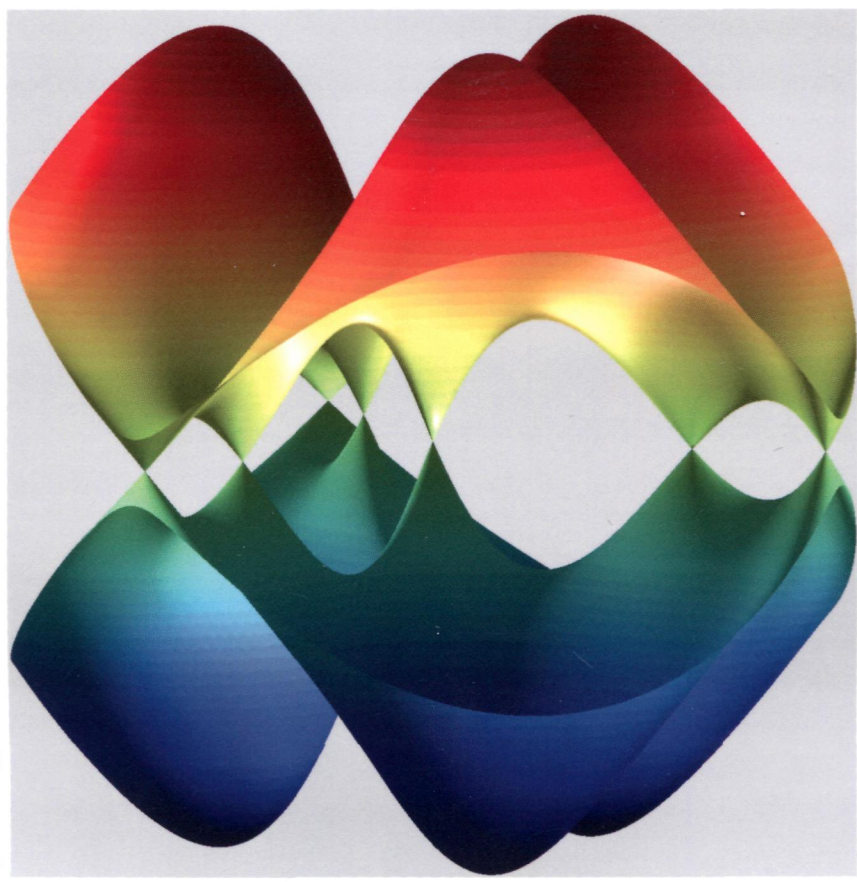


28 Apr

nu  
130/cp

Volume 140 Number 16

# AIP | The Journal of Chemical Physics



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



► Cover image from Mahesh B. Dawadi and David S. Perry, *J. Chem. Phys.* **140**, 161101 (2014).

## COMMUNICATIONS

- Communication: Conical intersections between vibrationally adiabatic surfaces in methanol (4 pages)**  
Mahesh B. Dawadi and David S. Perry ..... 161101
- Communication: On the origin of the surface term in the Ewald formula (4 pages)**  
V. Ballenegger ..... 161102
- Communication: Electron transfer mediated decay enabled by spin-orbit interaction in small krypton/xenon clusters (4 pages)**  
J. Patrick Zobel, Nikolai V. Kryzhevoi, and Markus Pernpointner ..... 161103
- Communication: Minimum in the thermal conductivity of supercooled water: A computer simulation study (4 pages)**  
F. Bresme, J. W. Biddle, J. V. Sengers, and M. A. Anisimov ..... 161104
- Communication: Spin-boson model with diagonal and off-diagonal coupling to two independent baths: Ground-state phase transition in the deep sub-Ohmic regime (4 pages)**  
Yang Zhao, Yao Yao, Vladimir Chernyak, and Yang Zhao ..... 161105
- Communication: Radial distribution functions in a two-dimensional binary colloidal hard sphere system (5 pages)**  
Alice L. Thorneywork, Roland Roth, Dirk G. A. L. Aarts, and Roel P. A. Dullens ..... 161106
- Communication: Atomic force detection of single-molecule nonlinear optical vibrational spectroscopy (5 pages)**  
Prasoon Saurabh and Shaul Mukamel ..... 161107

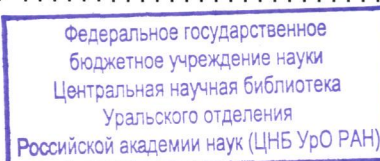
## ARTICLES

### Theoretical Methods and Algorithms

- Resummed thermodynamic perturbation theory for bond cooperativity in associating fluids with small bond angles: Effects of steric hindrance and ring formation (8 pages)**  
Bennett D. Marshall, Amin Haghmoradi, and Walter G. Chapman ..... 164101
- Charge transfer excitations from excited state Hartree-Fock subsequent minimization scheme (6 pages)**  
Iris Theophilou, M. Tassi, and S. Thanos ..... 164102
- Describing long-range charge-separation processes with subsystem density-functional theory (14 pages)**  
Alisa Solovyeva, Michele Pavanello, and Johannes Neugebauer ..... 164103
- Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: Explicit treatment of the vibronic transitions (6 pages)**  
Marco D'Abramo, Massimiliano Aschi, and Andrea Amadei ..... 164104
- Electron dynamics in complex environments with real-time time dependent density functional theory in a QM-MM framework (9 pages)**  
Uriel N. Morzan, Francisco F. Ramírez, M. Belén Oviedo, Cristián G. Sánchez, Damián A. Scherlis, and Mariano C. González Lebrero ..... 164105

(Continued)

A1



© 2014 AIP Publishing LLC

<b>Assessing the accuracy of the isotropic periodic sum method through Madelung energy computation (4 pages)</b> Pedro Ojeda-May and Jingzhi Pu .....	164106
<b>Vibrational solvatochromism. II. A first-principle theory of solvation-induced vibrational frequency shift based on effective fragment potential method (16 pages)</b> Bartosz Błasiak and Minhaeng Cho .....	164107
<b>Calculation of state-to-state cross sections for triatomic reaction by the multi-configuration time-dependent Hartree method (8 pages)</b> Bin Zhao, Dong-H. Zhang, Soo-Y. Lee, and Zhigang Sun .....	164108
<b>Sampling saddle points on a free energy surface (9 pages)</b> Amit Samanta, Ming Chen, Tang-Qing Yu, Mark Tuckerman, and Weinan E .....	164109
<b>Two-level system in spin baths: Non-adiabatic dynamics and heat transport (11 pages)</b> Dvira Segal .....	164110
<b>Development of multicomponent hybrid density functional theory with polarizable continuum model for the analysis of nuclear quantum effect and solvent effect on NMR chemical shift (6 pages)</b> Yusuke Kanematsu and Masanori Tachikawa .....	164111
<b>Constructing polyatomic potential energy surfaces by interpolating diabatic Hamiltonian matrices with demonstration on green fluorescent protein chromophore (13 pages)</b> Jae Woo Park and Young Min Rhee .....	164112
<b>Local CC2 response method based on the Laplace transform: Analytic energy gradients for ground and excited states (16 pages)</b> Katrin Ledermüller and Martin Schütz .....	164113
<b>The cavity electromagnetic field within the polarizable continuum model of solvation (16 pages)</b> Silvio Pipolo, Stefano Corni, and Roberto Cammi .....	164114
<b>A finite difference Davidson procedure to sidestep full <i>ab initio</i> hessian calculation: Application to characterization of stationary points and transition state searches (9 pages)</b> Shaama Mallikarjun Sharada, Alexis T. Bell, and Martin Head-Gordon .....	164115
<b>Static correlation beyond the random phase approximation: Dissociating H<sub>2</sub> with the Bethe-Salpeter equation and time-dependent GW (14 pages)</b> Thomas Olsen and Kristian S. Thygesen .....	164116

### Advanced Experimental Techniques

<b>Quantification of pore size distribution using diffusion NMR: Experimental design and physical insights (16 pages)</b> Yaniv Katz and Uri Nevo .....	164201
--	--------

### Atoms, Molecules, and Clusters

<b>Atomic shell structure from the Single-Exponential Decay Detector (8 pages)</b> Piotr de Silva, Jacek Korchowiec, and Tomasz A. Wesolowski .....	164301
<b>An experimental and <i>ab initio</i> study of the electronic spectrum of the jet-cooled F<sub>2</sub>BO free radical (8 pages)</b> Robert Grimminger, Phillip M. Sheridan, and Dennis J. Clouthier .....	164302
<b>Interpretation of the accidental predissociation of the E<sup>1</sup> Π state of CO (8 pages)</b> M. Majumder, N. Sathyamurthy, G. J. Vázquez, and H. Lefebvre-Brion .....	164303
<b>Dissociation dynamics of simple chlorine containing molecules upon resonant Cl K-σ<sup>*</sup> excitation (7 pages)</b> R. Bohinc, M. Žitnik, K. Bučar, and M. Kavčič .....	164304

<b>Experimental nanocalorimetry of protonated and deprotonated water clusters (7 pages)</b> Julien Boulon, Isabelle Braud, Sébastien Zamith, Pierre Labastie, and Jean-Marc L'Hermite .....	164305
<b>Confinement induced binding of noble gas atoms (11 pages)</b> Munmun Khatua, Sudip Pan, and Pratim K. Chattaraj .....	164306
<b>Photoisomerization action spectrum of retinal protonated Schiff base in the gas phase (10 pages)</b> N. J. A. Coughlan, K. J. Catani, B. D. Adamson, U. Wille, and E. J. Bieske .....	164307
<b>Scattering matrix approach to the dissociative recombination of HCO<sup>+</sup> and N<sub>2</sub>H<sup>+</sup> (12 pages)</b> S. Fonseca dos Santos, N. Douguet, V. Kokoouline, and A. E. Orel .....	164308
<b>Time-dependent restricted-active-space self-consistent-field singles method for many-electron dynamics (6 pages)</b> Haruhide Miyagi and Lars Bojer Madsen .....	164309
<b>Anharmonic coupling between fundamental modes in tetramethylurea (5 pages)</b> Yuanzheng Chen, Zhiwei Men, Juntao Li, Zhanlong Li, Shengnan Sun, Chengling Sun, Shuqin Gao, Zuowei Li, and Mi Zhou .....	164310
<b>High resolution jet-cooled infrared absorption spectra of the formic acid dimer: A reinvestigation of the C–O stretch region (6 pages)</b> Kusse G. Goroya, Yu Zhu, Ping Sun, and Chuanxi Duan .....	164311
<b>Spectroscopic and thermodynamic properties of molecular hydrogen dissolved in water at pressures up to 200 MPa (8 pages)</b> Jacek Borysow, Leonardo del Rosso, Milva Celli, Massimo Moraldi, and Lorenzo Ulivi .....	164312
<b>Influence of spin-orbit effects on structures and dielectric properties of neutral lead clusters (6 pages)</b> D. A. Götz, A. Shayeghi, R. L. Johnston, P. Schwerdtfeger, and R. Schäfer .....	164313
<b>Laser induced rovibrational cooling of the linear polyatomic ion C<sub>2</sub>H<sub>2</sub><sup>+</sup> (13 pages)</b> Nabanita Deb, Brianna R. Heazlewood, Christopher J. Rennick, and Timothy P. Softley .....	164314
<b>Theoretical calculations and vibrational potential energy surface of 4-silaspiro(3,3)heptane (5 pages)</b> Esther J. Ocola, Cross Medders, Niklas Meinander, and Jaan Laane .....	164315
<b>The PtAl<sup>-</sup> and PtAl<sub>2</sub><sup>-</sup> anions: Theoretical and photoelectron spectroscopic characterization (4 pages)</b> Xinxing Zhang, Gerd Ganteför, Kit H. Bowen, and Anastassia N. Alexandrova .....	164316
<b>Photoelectron spectroscopy of boron aluminum hydride cluster anions (8 pages)</b> Haopeng Wang, Xinxing Zhang, Yeon Jae Ko, Gerd Gantefoer, Kit H. Bowen, Xiang Li, Boggavarapu Kiran, and Anil K. Kandalam .....	164317

### Liquids, Glasses, and Crystals

<b>Onset of simple liquid behaviour in modified water models (11 pages)</b> Saurav Prasad and Charusita Chakravarty .....	164501
<b>Intermittent dynamics and logarithmic domain growth during the spinodal decomposition of a glass-forming liquid (17 pages)</b> Vincent Testard, Ludovic Berthier, and Walter Kob .....	164502
<b>Correlation between thermodynamic anomalies and pathways of ice nucleation in supercooled water (8 pages)</b> Rakesh S. Singh and Biman Bagchi .....	164503
<b>Inelastic incoherent neutron scattering study of the molecular properties of pure hydrogen peroxide and its water mixtures of different concentration (10 pages)</b> Peter W. Albers, Jürgen Glenneberg, Keith Refson, and Stewart F. Parker .....	164504
<b>Catalytic activity of methanol in all-vapor subsecond clathrate-hydrate formation (7 pages)</b> J. Paul Devlin .....	164505



<b>Two-component order parameter for quantifying clathrate hydrate nucleation and growth</b> (6 pages) Brian C. Barnes, Gregg T. Beckham, David T. Wu, and Amadeu K. Sum	164506
<b>Channel flow of a tensorial shear-thinning Maxwell model: Lattice Boltzmann simulations</b> (13 pages) S. Papenkort and Th. Voigtmann	164507
<b>Thermal equation of state of solid naphthalene to 13 GPa and 773 K: <i>In situ</i> X-ray diffraction study and first principles calculations</b> (8 pages) Anna Y. Likhacheva, Sergey V. Rashchenko, Artem D. Chanyshhev, Talgat M. Inerbaev, Konstantin D. Litasov, and Dmitry S. Kilin	164508
<b>The Raman spectrum of CaCO<sub>3</sub> polymorphs calcite and aragonite: A combined experimental and computational study</b> (12 pages) Marco De La Pierre, Cédric Carteret, Lorenzo Maschio, Erwan André, Roberto Orlando, and Roberto Dovesi	164509
<b>Quadrupole terms in the Maxwell equations: Debye-Hückel theory in quadrupolarizable solvent and self-salting-out of electrolytes</b> (12 pages) Radomir I. Slavchov	164510
<b><i>Ab initio</i> calculation of the electronic absorption spectrum of liquid water</b> (9 pages) Hugo F. M. C. Martiniano, Nuno Galamba, and Benedito J. Costa Cabral	164511
<b>Probing the interplay between electrostatic and dispersion interactions in the solvation of nonpolar nonaromatic solute molecules in ionic liquids: An OKE spectroscopic study of CS<sub>2</sub>/[C<sub>n</sub>C<sub>1</sub>im][NTf<sub>2</sub>] mixtures (n = 1–4)</b> (11 pages) Lianjie Xue, George Tamas, Eshan Gurung, and Edward L. Quitevis	164512
<b>Surfaces, Interfaces, and Materials</b>	
<b>Surface forces: Surface roughness in theory and experiment</b> (10 pages) Drew F. Parsons, Rick B. Walsh, and Vincent S. J. Craig	164701
<b>Mechanism of oil detachment from hybrid hydrophobic and hydrophilic surface in aqueous solution</b> (10 pages) Peili Zhang, Zhen Xu, Qian Liu, and Shiling Yuan	164702
<b>Negative differential resistance devices by using N-doped graphene nanoribbons</b> (7 pages) Jing Huang, Weiyi Wang, Qunxiang Li, and Jinlong Yang	164703
<b>Phase stability limit of c-BN under hydrostatic and non-hydrostatic pressure conditions</b> (7 pages) Jianwei Xiao, Jinglian Du, Bin Wen, Roderick Melnik, Yoshiyuki Kawazoe, and Xiangyi Zhang	164704
<b>Do Ag<sub>n</sub> (up to n = 8) clusters retain their identity on graphite? Insights from first-principles calculations including dispersion interactions</b> (8 pages) Akansha Singh, Chiranjib Majumder, and Prasenjit Sen	164705
<b>Pressure-induced ferroelastic phase transition in SnO<sub>2</sub> from density functional theory</b> (5 pages) Lei Yang, Weiliu Fan, Yanlu Li, Lei Wei, and Xian Zhao	164706
<b>A model for the latent heat of melting in free standing metal nanoparticles</b> (5 pages) Jeong-Heon Shin and Mark R. Deinert	164707
<b>Periodic ordering of clusters and stripes in a two-dimensional lattice model. II. Results of Monte Carlo simulation</b> (12 pages) N. G. Almarza, J. Pękalski, and A. Ciach	164708
<b>The different roles of Pu-oxide overlayers in the hydrogenation of Pu-metal: An <i>ab initio</i> molecular dynamics study based on van der Waals density functional (vdW-DF)+U</b> (13 pages) Bo Sun, Haifeng Liu, Haifeng Song, Guangcai Zhang, Hui Zheng, Xian-Geng Zhao, and Ping Zhang	164709

**Near-edge X-ray absorption fine-structure spectroscopy of naphthalene diimide-thiophene co-polymers (8 pages)**

Eliot Gann, Christopher R. McNeill, Monika Szumilo, Henning Sirringhaus, Michael Sommer, Subashani Maniam, Steven J. Langford, and Lars Thomsen ..... 164710

**Predicting for thermodynamic instabilities in water/oil/surfactant microemulsions: A mesoscopic modelling approach (11 pages)**

Magali Duvail, Lise Arleth, Thomas Zemb, and Jean-François Dufrêche ..... 164711

**Polymers and Soft Matter****Homogeneous states in driven granular mixtures: Enskog kinetic theory versus molecular dynamics simulations (10 pages)**

Nagi Khalil and Vicente Garzó ..... 164901

**Hydrodynamic radius approximation for spherical particles suspended in a viscous fluid:****Influence of particle internal structure and boundary (7 pages)**

Bogdan Cichocki, Maria L. Ekiel-Jeżewska, and Eligiusz Wajnryb ..... 164902

**Diradicals acting through diamagnetic phenylene vinylene bridges: Raman spectroscopy as a probe to characterize spin delocalization (9 pages)**

Sandra Rodríguez González, Belén Nieto-Ortega, Rafael C. González Cano, Vega Lloveras, Juan J. Novoa, Fernando Mota, José Vidal-Gancedo, Concepció Rovira, Jaume Veciana, Elena del Corro, Mercedes Taravillo, Valentín G. Baonza, Juan T. López Navarrete, and Juan Casado ..... 164903

**Lattice-Boltzmann simulations of the electrophoretic stretching of polyelectrolytes: The importance of hydrodynamic interactions (7 pages)**

Owen A. Hickey, Christian Holm, and Jens Smiatek ..... 164904

**Mixtures composed of liquid crystals and carbon nanotubes (9 pages)**

V. Popa-Nita ..... 164905

**Electrostatic interaction between colloidal particles trapped at an electrolyte interface (5 pages)**

Arghya Majee, Markus Bier, and S. Dietrich ..... 164906

**Biological Molecules and Networks****Hydration of non-polar anti-parallel  $\beta$ -sheets (6 pages)**

Tomaz Urbic and Cristiano L. Dias ..... 165101

**LETTERS TO THE EDITOR****Comments****Comment on "Effective field parameters in iron Mössbauer spectroscopy"**

[J. Chem. Phys. 47, 961 (1967)] (2 pages)

W. N. Rowan-Weetaluktuk, J. M. Cadogan, and D. H. Ryan ..... 167101

**Errata****Erratum: "Conservative and dissipative force field for simulation of coarse-grained alkane molecules: A bottom-up approach" [J. Chem. Phys. 140, 134113 (2014)] (1 page)**

Sébastien Trément, Benoît Schnell, Laurent Petitjean, Marc Couty, and Bernard Rousseau ..... 169901

**Erratum: "Crossing the dividing surface of transition state theory. I. Underlying symmetries and motion coordination in multidimensional systems" [J. Chem. Phys. 140, 134303 (2014)] (1 page)** 169902  
 J. C. Lorquet

**Erratum: "Free-energy analysis of water affinity in polymer studied by atomistic molecular simulation combined with the theory of solutions in the energy representation" [J. Chem. Phys. 137, 234903 (2012)] (2 pages)** 169903  
 Tomonori Kawakami, Isamu Shigemoto, and Nobuyuki Matubayasi