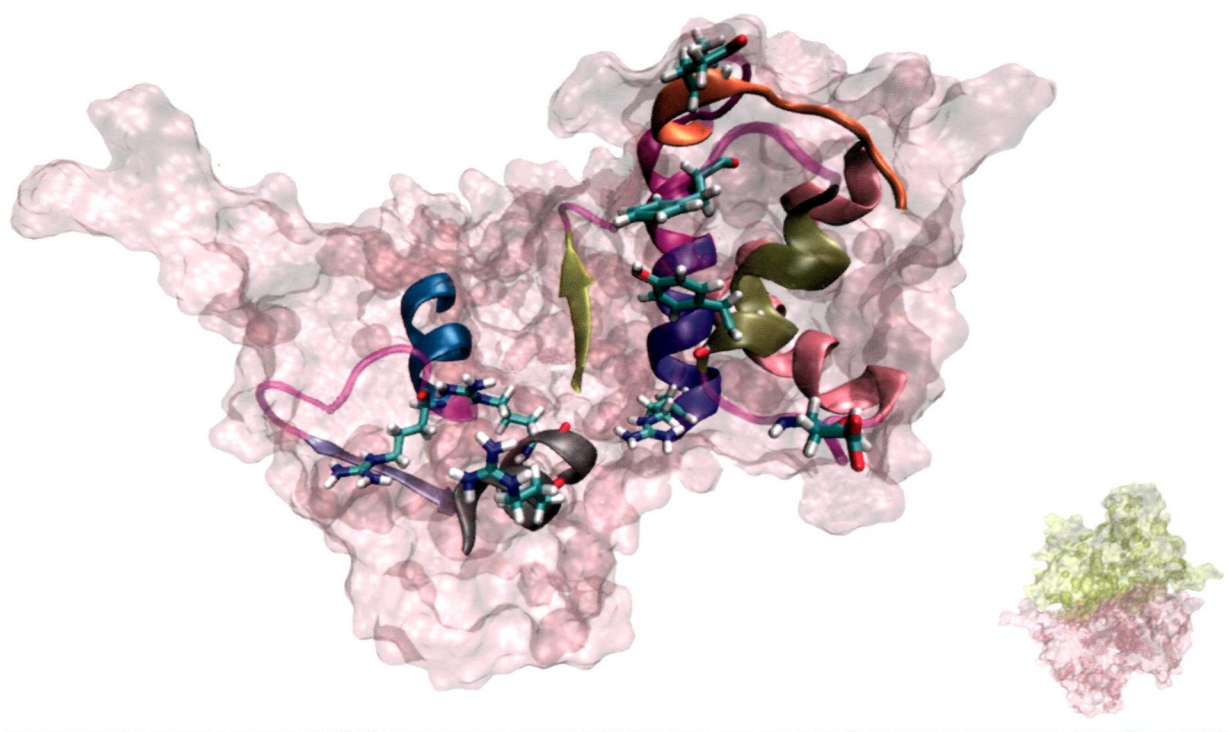


ПН
J80/CP

14 December 2013

Volume 139 Number 22

AIP | The Journal of Chemical Physics



jcp.aip.org

80th
Anniversary

► Cover image from Shan-Yan Chang, Fu-Feng Liu, Xiao-Yan Dong, and Yan Sun, *J. Chem. Phys.* **139**, 225102 (2013).

COMMUNICATIONS

- Communication: A new paradigm for structure prediction in multicomponent systems (4 pages)**
D. Schebarchov and D. J. Wales 221101
- Communication: Angular momentum alignment and fluorescence polarization of alkali atoms photodetached from helium nanodroplets (4 pages)**
Alberto Hernando, J. Alberto Beswick, and Nadine Halberstadt 221102
- Communication: Theoretical study of ThO for the electron electric dipole moment search (4 pages)**
L. V. Skripnikov, A. N. Petrov, and A. V. Titov 221103

ARTICLES

Theoretical Methods and Algorithms

- Tensor decomposition in post-Hartree–Fock methods. II. CCD implementation (10 pages)**
Udo Benedikt, Karl-Heinz Böhm, and Alexander A. Auer 224101
- Approaching the complete-basis limit with a truncated many-body expansion (11 pages)**
Ryan M. Richard, Ka Un Lao, and John M. Herbert 224102
- Wavelet analysis of molecular dynamics: Efficient extraction of time-frequency information in ultrafast optical processes (9 pages)**
Javier Prior, Enrique Castro, Alex W. Chin, Javier Almeida, Susana F. Huelga, and Martin B. Plenio 224103
- Orbital-free bond breaking via machine learning (10 pages)**
John C. Snyder, Matthias Rupp, Katja Hansen, Leo Blooston, Klaus-Robert Müller, and Kieron Burke 224104
- Double, Rydberg and charge transfer excitations from pairing matrix fluctuation and particle-particle random phase approximation (6 pages)**
Yang Yang, Helen van Aggelen, and Weitao Yang 224105
- Ensemble simulations with discrete classical dynamics (8 pages)**
Søren Toxvaerd 224106
- Domain of validity of the perturbative approach to femtosecond optical spectroscopy (8 pages)**
Maxim F. Gelin, B. Jayachander Rao, Mathias Nest, and Wolfgang Domcke 224107
- The weak-correlation limits of few-electron harmonium atoms (5 pages)**
Jerzy Cioslowski 224108
- The fluctuation-dissipation theorem for stochastic kinetics—Implications on genetic regulations (10 pages)**
Ching-Cher Sanders Yan and Chao-Ping Hsu 224109
- Excited electronic states from a variational approach based on symmetry-projected Hartree–Fock configurations (12 pages)**
Carlos A. Jiménez-Hoyos, R. Rodríguez-Guzmán, and Gustavo E. Scuseria 224110

- Time-dependent density functional theory quantum transport simulation in non-orthogonal basis (12 pages)**
 Yan Ho Kwok, Hang Xie, Chi Yung Yam, Xiao Zheng, and Guan Hua Chen 224111

- Criteria for the accuracy of small polaron quantum master equation in simulating excitation energy transfer dynamics (11 pages)**
 Hung-Tzu Chang, Pan-Pan Zhang, and Yuan-Chung Cheng 224112

Atoms, Molecules, and Clusters

- A new *ab initio* potential energy surface for the collisional excitation of HCN by para- and ortho-H₂ (8 pages)**
 Otoniel Denis-Alpizar, Yulia Kalugina, Thierry Stoecklin, Mario Hernández Vera, and François Lique 224301

- Anharmonic rovibrational calculations of singlet cyclic C₄ using a new *ab initio* potential and a quartic force field (7 pages)**
 Xiaohong Wang, Xinchuan Huang, Joel M. Bowman, and Timothy J. Lee 224302

- Approximate photochemical dynamics of azobenzene with reactive force fields (9 pages)**
 Yan Li and Bernd Hartke 224303

- Rotational spectroscopy of pyridazine and its isotopologs from 235–360 GHz: Equilibrium structure and vibrational satellites (13 pages)**
 Brian J. Esselman, Brent K. Amberger, Joshua D. Shutter, Mitchell A. Daane, John F. Stanton, R. Claude Woods, and Robert J. McMahon 224304

- Ionic liquids from the bottom up: Local assembly motifs in [EMIM][BF₄] through cryogenic ion spectroscopy (7 pages)**
 Christopher J. Johnson, Joseph A. Fournier, Conrad T. Wolke, and Mark A. Johnson 224305

- The stability of S-states of unit-charge Coulomb three-body systems: From H⁻ to H₂⁺ (7 pages)**
 Andrew W. King, Frank Longford, and Hazel Cox 224306

- Three-chain B_{6n+14} cages as possible precursors for the syntheses of boron fullerenes (5 pages)**
 Haigang Lu and Si-Dian Li 224307

- Combined photoelectron, collision-induced dissociation, and computational studies of parent and fragment anions of *N*-paranitrophenylsulfonylethylalanine and *N*-paranitrophenylalanine (9 pages)**
 Jason Lambert, Jing Chen, Angela Buonaugurio, Kit H. Bowen, Chi-Linh Do-Thanh, Yilin Wang, Michael D. Best, R. N. Compton, and Thomas Sommerfeld 224308

- On the origin of high transient anisotropies: An exemplification in a Cd-porphyrin (6 pages)**
 Yu Liang, Melanie Klinger, Oliver Schalk, and Andreas-Neil Unterreiner 224309

- Competition between abstraction and exchange channels in H + HCN reaction: Full-dimensional quantum dynamics (7 pages)**
 Bin Jiang and Hua Guo 224310

- Global reaction route mapping of isomerization pathways of exotic C₆H molecular species (13 pages)**
 Vikas and Gurpreet Kaur 224311

Liquids, Glasses, and Crystals

- Critical anomalies of alkaline fading of phenolphthalein in the critical solution of 2-butoxyethanol + water (7 pages)**
 Zhongyu Du, Handi Yin, Zhiguo Hao, Peizhu Zheng, and Weiguo Shen 224501

- Insights on cholinium- and piperazinium-based ionic liquids under external electric fields: A molecular dynamics study (13 pages)**
 Santiago Aparicio, Mert Atilhan, and Nezih Pala 224502

(Continued)

Regimes of streaming potential in cylindrical nano-pores in presence of finite sized ions and charge induced thickening: An analytical approach (13 pages) Aditya Bandopadhyay, Prakash Goswami, and Suman Chakraborty	224503
Revisiting dynamics near a liquid-liquid phase transition in Si and Ga: The fragile-to-strong transition (7 pages) Samuel Cajahuaringa, Maurice de Koning, and Alex Antonelli	224504

Surfaces, Interfaces, and Materials

Surface structures of binary mixtures of imidazolium-based ionic liquids using high-resolution Rutherford backscattering spectroscopy and time of flight secondary ion mass spectroscopy (8 pages) Kaoru Nakajima, Motoki Miyashita, Motofumi Suzuki, and Kenji Kimura	224701
Strain effect on the adsorption, diffusion, and molecular dissociation of hydrogen on Mg (0001) surface (8 pages) Huaping Lei, Caizhuang Wang, Yongxin Yao, Yangang Wang, Myron Hupalo, Dan McDougall, Michael Tringides, and Kaiming Ho	224702
Temperature dependence of the crystal-liquid interfacial free energy and the endpoint of the melting line (11 pages) Vladimir G. Baidakov, Sergey P. Protsenko, and Azat O. Tipseev	224703
Binding and interlayer force in the near-contact region of two graphite slabs: Experiment and theory (6 pages) Tim Gould, Ze Liu, Jefferson Zhe Liu, John F. Dobson, Quanshui Zheng, and S. Lebègue	224704
A first-principles study of structural and elastic properties of bulk SrRuO₃ (12 pages) Š. Masys and V. Jonauskas	224705
Parallel kinetic Monte Carlo simulation framework incorporating accurate models of adsorbate lateral interactions (13 pages) Jens Nielsen, Mayeul d'Avezac, James Hetherington, and Michail Stamatakis	224706
High-resolution neutron diffraction study of CuNCN: New evidence of structure anomalies at low temperature (5 pages) Philipp Jacobs, Andreas Houben, Andrei L. Tchougréeff, and Richard Dronskowski	224707
Spin-polarized hydrogen adsorbed on the surface of superfluid ⁴He (6 pages) J. M. Marín, L. Vranješ Markić, and J. Boronat	224708
Enantioselectivity of (321) chiral noble metal surfaces: A density functional theory study of lactate adsorption (5 pages) J.-H. Franke and D. S. Kosov	224709
The relationship between local liquid density and force applied on a tip of atomic force microscope: A theoretical analysis for simple liquids (7 pages) Ken-ichi Amano, Kazuhiro Suzuki, Takeshi Fukuma, Ohgi Takahashi, and Hiroshi Onishi	224710
Fluid of Janus molecules between two walls: The solvation force (9 pages) A. Patrykiewicz, S. Sokołowski, Z. Sokołowska, and Ja. Ilnytskyi	224711

Polymers and Soft Matter

Phase diagrams of block copolymer melts by dissipative particle dynamics simulations (10 pages) Alexey A. Gavrilov, Yaroslav V. Kudryavtsev, and Alexander V. Chertovich	224901
Dynamics of a polyelectrolyte in simple shear flow (11 pages) Kandiledath Jayasree, Raj Kumar Manna, Debapriya Banerjee, and P. B. Sunil Kumar	224902

Some aspects of the orientational order distribution of flexible chains in a diblock mesophase (9 pages) Cédric Lorthioir, Solo Randriamahefa, and Bertrand Deloche	224903
A percolation-based model for the conductivity of nanofiber composites (6 pages) Avik P. Chatterjee	224904
Structure factor of model bidisperse ferrofluids with relatively weak interparticle interactions (14 pages) Ekaterina Novak, Elena Minina, Elena Pyanzina, Sofia Kantorovich, and Alexey Ivanov	224905
The entropy of the rotational conformations of (poly)isoprene molecules and its relationship to rubber elasticity and temperature increase for moderate tensile or compressive strains (7 pages) David E. Hanson, John L. Barber, and Gopinath Subramanian	224906

Biological Molecules and Networks

Volume properties and spectroscopy: A terahertz Raman investigation of hen egg white lysozyme (7 pages) Paola Sassi, Stefania Perticaroli, Lucia Comez, Alessandra Giugliarelli, Marco Paolantoni, Daniele Fioretto, and Assunta Morresi	225101
Molecular insight into conformational transmission of human P-glycoprotein (12 pages) Shan-Yan Chang, Fu-Feng Liu, Xiao-Yan Dong, and Yan Sun	225102
Structural flexibility of intrinsically disordered proteins induces stepwise target recognition (10 pages) Nobu C. Shirai and Macoto Kikuchi	225103
The eigenmode perspective of NMR spin relaxation in proteins (14 pages) Yury E. Shapiro and Eva Meirovitch	225104
Reorientation of the helix of the tryptophan-rich gp41W peptide from HIV-1 at interfaces (8 pages) Gladys Matar, Emmanuel Benichou, Mehmet Nail Nasir, Yara El Harfouch, Pierre-François Brevet, and Françoise Besson	225105

LETTERS TO THE EDITOR

Errata

Publisher's Note: "Molecular recognition of DNA by ligands: Roughness and complexity of the free energy profile" [J. Chem. Phys. 139, 145102 (2013)] (1 page) Wenwei Zheng, Attilio Vittorio Vargiu, Mary A. Rohrdanz, Paolo Carloni, and Cecilia Clementi	229901
Erratum: "MuSTAR MD: Multi-scale sampling using temperature accelerated and replica exchange molecular dynamics" [J. Chem. Phys. 139, 145105 (2013)] (1 page) Yu Yamamori and Akio Kitao	229902
Erratum: "Unitary group adapted state-specific multi-reference coupled cluster theory: Formulation and pilot numerical applications" [J. Chem. Phys. 137, 024105 (2012)] (2 pages) Rahul Maitra, Debalina Sinha, and Debashis Mukherjee	229903