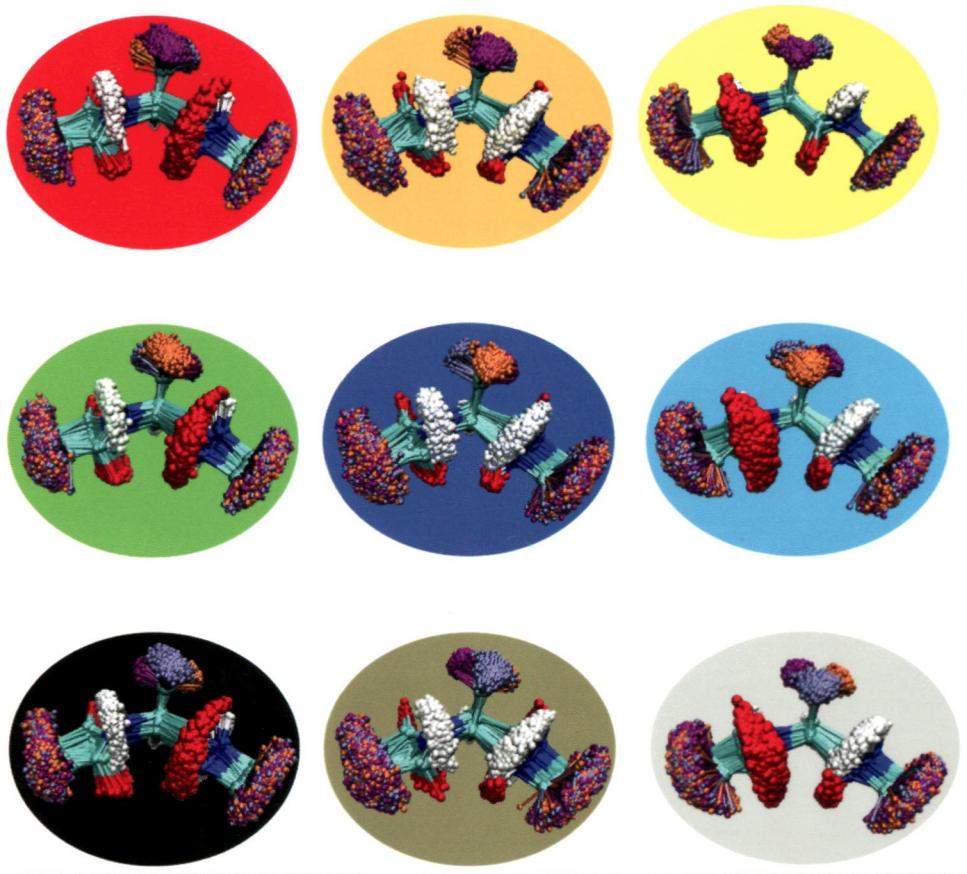


NU
J80/cp 2013

Volume 139 Number 17

AIP | The Journal of Chemical Physics



80th
Anniversary

jcp.aip.org

► Cover image from *Zheng Yi, Benjamin Lindner, Jan-Hendrik Prinz, Frank Noé, and Jeremy C. Smith, J. Chem. Phys.* **139**, 175102 (2013).

COMMUNICATIONS

Communication: The Rosenfeld-Tarazona expression for liquids' specific heat: A numerical investigation of eighteen systems (4 pages)

Trond S. Ingebrigtsen, Arno A. Veldhorst, Thomas B. Schröder, and Jeppe C. Dyre 171101

Communication: Transfer ionization in a thermal reaction of a cation and anion:

Ar^+ with Br^- and I^- (3 pages)

Nicholas S. Shuman, Thomas M. Miller, Rainer Johnsen,
and Albert A. Viggiano 171102

Communication: Random phase approximation renormalized many-body perturbation theory (4 pages)

Jefferson E. Bates and Filipp Furche 171103

ARTICLES

Theoretical Methods and Algorithms

A simple monomer-based model-Hamiltonian approach to combine excitonic coupling and Jahn-Teller theory (11 pages)

Pablo García-Fernández, Ljubica Andjelković, Matija Zlatar, Maja Gruden-Pavlović,
and Andreas Dreuw 174101

Tractability gains in symmetry-adapted perturbation theory including coupled double excitations: CCD+ST(CCD) dispersion with natural orbital truncations (15 pages)

Robert M. Parrish, Edward G. Hohenstein, and C. David Sherrill 174102

Massively parallel implementations of coupled-cluster methods for electron spin resonance spectra. I. Isotropic hyperfine coupling tensors in large radicals (12 pages)

Prakash Verma, Ajith Perera, and Jorge A. Morales 174103

A multireference perturbation method using non-orthogonal Hartree-Fock determinants for ground and excited states (9 pages)

Shane R. Yost, Tim Kowalczyk, and Troy Van Voorhis 174104

Analyzing milestone networks for molecular kinetics: Definitions, algorithms, and examples (17 pages)

Shruthi Viswanath, Steven M. Kreuzer, Alfredo E. Cardenas, and Ron Elber 174105

A comparison of geometric parameters from PBE-based doubly hybrid density functionals PBE0-DH, PBE0-2, and xDH-PBE0 (11 pages)

Neil Qiang Su, Carlo Adamo, and Xin Xu 174106

Zero-multipole summation method for efficiently estimating electrostatic interactions in molecular system (14 pages)

Ikuo Fukuda 174107

Mixed quantum/classical theory of rotationally and vibrationally inelastic scattering in space-fixed and body-fixed reference frames (15 pages)

Alexander Semenov and Dmitri Babikov 174108

Quantized Hamiltonian dynamics captures the low-temperature regime of charge transport in molecular crystals (10 pages)	Linjun Wang, Alexey V. Akimov, Liping Chen, and Oleg V. Prezhdo	174109
Benchmark tests and spin adaptation for the particle-particle random phase approximation (10 pages)	Yang Yang, Helen van Aggelen, Stephan N. Steinmann, Degao Peng, and Weitao Yang	174110
Block correlated second order perturbation theory with a generalized valence bond reference function (10 pages)	Enhua Xu and Shuhua Li	174111
Atoms, Molecules, and Clusters		
Pi and sigma double conjugations in boronyl polyboroene nanoribbons: $B_n(BO)_2^-$ and $B_n(BO)_2$ ($n = 5-12$) (7 pages)	Hua-Jin Zhai, Qiang Chen, Hui Bai, Hai-Gang Lu, Wei-Li Li, Si-Dian Li, and Lai-Sheng Wang	174301
Relative energies, structures, vibrational frequencies, and electronic spectra of pyrylium cation, an oxygen-containing carbocyclic ring isoelectronic with benzene, and its isomers (9 pages)	Partha P. Bera, Martin Head-Gordon, and Timothy J. Lee	174302
Time domain simulations of chemical bonding effects in surface-enhanced spectroscopy (5 pages)	Patrick Z. El-Khoury, Eric J. Bylaska, and Wayne P. Hess	174303
Mass-resolved two-photon and photoelectron spectra of ArXe in the region of $Xe^+ 7p, 6p'$, 6d (10 pages)	L. P. Rakcheeva, P. Yu. Serdobintsev, A. A. Belyaeva, I. A. Shevkunov, A. S. Melnikov, A. A. Nakozina, A. A. Pastor, and M. A. Khodorkovskii	174304
Photodissociation mechanisms of the CO_2^{2+} dication studied using multi-state multiconfiguration second-order perturbation theory (11 pages)	Dongwen Zhang, Bo-Zhen Chen, Ming-Bao Huang, Qingyong Meng, and Zhiyuan Tian	174305
An experimental and theoretical study of the electronic spectrum of HPS, a second row HNO analog (12 pages)	Robert Grimminger, Dennis J. Clouthier, Riccardo Tarroni, Zhong Wang, and Trevor J. Sears	174306
Thiol-based molecular overlayers adsorbed on C_{60}: Role of the end-group and charge state on the stability of the complexes (11 pages)	R. Chavira-Quintero and R. A. Guirado-López	174307
The structure of mixed $^3He-^4He$ droplets doped with OCS: A density functional approach (6 pages)	Antonio Leal, David Mateo, Martí Pi, Manuel Barranco, and Jesús Navarro	174308
First-principles prediction of magnetic superatoms in 4d-transition-metal-doped magnesium clusters (8 pages)	Gui-Xian Ge, Yan Han, Jian-Guo Wan, Ji-Jun Zhao, and Guang-Hou Wang	174309
Benzene analogues of (quasi-)planar $M@B_nH_n$ compounds ($M = V^-, Cr, Mn^+$): A theoretical investigation (7 pages)	Lifen Li (李丽芬), Chang Xu (徐畅), Baokang Jin (金葆康), and Longjiu Cheng (程龙玖)	174310
Binary nucleation rates for ethanol/water mixtures in supersonic Laval nozzles: Analyses by the first and second nucleation theorems (18 pages)	Shinobu Tanimura, Harshad Pathak, and Barbara E. Wyslouzil	174311
IR mass-resolved spectroscopy of complexes without chromophore: Cyclohexanol · $(H_2O)_n$, $n = 1-3$ and cyclohexanol dimer (10 pages)	Iker León, Raúl Montero, Asier Longarte, and José A. Fernández	174312

Ab initio structural and spectroscopic study of HPS^x and HSP^x (x = 0,+1,-1) in the gas phase (12 pages)	
Saida Ben Yaghlane, C. Eric Cotton, Joseph S. Francisco, Roberto Lingerri, and Majdi Hochlaf	174313
Site-dependent Si KL₂₃L₂₃ resonant Auger electron spectra following inner-shell excitation of Cl₃SiSi(CH₃)₃ (7 pages)	
Isao H. Suzuki, Hikari Endo, Kanae Nagai, Osamu Takahashi, Yusuke Tamenori, and Shin-ichi Nagaoka	174314
Nuclear quantum effects on the structure and the dynamics of [H₂O]₈ at low temperatures (9 pages)	
Pablo E. Videla, Peter J. Rossky, and D. Laria	174315
Spectroscopy and applications of the 3³Σ⁺ electronic state of ³⁹K⁸⁵Rb (8 pages)	
Jayita Banerjee, David Rahmlow, Ryan Carollo, Michael Bellos, Edward E. Eyler, Phillip L. Gould, and William C. Stwalley	174316
Dynamics of carbon-hydrogen and carbon-methyl exchanges in the collision of ³P atomic carbon with propene (10 pages)	
Shih-Huang Lee, Wei-Kan Chen, Chih-Hao Chin, and Wen-Jian Huang	174317
The pure rotational spectrum of ruthenium monocarbide, RuC, and relativistic <i>ab initio</i> predictions (6 pages)	
Fang Wang, Timothy C. Steimle, Allan G. Adam, Lan Cheng, and John F. Stanton	174318

Liquids, Glasses, and Crystals

Pressure dependent stability and structure of carbon dioxide—A density functional study including long-range corrections (8 pages)	
Sebastian Gohr, Stefan Grimme, Tilo Söhnel, Beate Paulus, and Peter Schwerdtfeger	174501
Size distribution of associated clusters in liquid alcohols: Interpretation of simulation results in the frame of SAFT approach (9 pages)	
Jiří Janeček and Patrice Paricaud	174502
A computational investigation of attrition-enhanced chiral symmetry breaking in conglomerate crystals (12 pages)	
Francesco Ricci, Frank H. Stillinger, and Pablo G. Debenedetti	174503
Interactions in ion pairs of protic ionic liquids: Comparison with aprotic ionic liquids (9 pages)	
Seiji Tsuzuki, Wataru Shinoda, Md. Shah Miran, Hiroshi Kinoshita, Tomohiro Yasuda, and Masayoshi Watanabe	174504
Liquid to solid nucleation via onion structure droplets (8 pages)	
Kipton Barros and W. Klein	174505
Internal friction of hydrated soda-lime-silicate glasses (6 pages)	
S. Reinsch, R. Müller, J. Deubener, and H. Behrens	174506

Surfaces, Interfaces, and Materials

Large work function reduction by adsorption of a molecule with a negative electron affinity: Pyridine on ZnO(10̄10) (10 pages)	
Oliver T. Hofmann, Jan-Christoph Deinert, Yong Xu, Patrick Rinke, Julia Stähler, Martin Wolf, and Matthias Scheffler	174701
A new (2 × 1) dimerized structure of monolayer 1T-molybdenum disulfide, studied from first principles calculations (7 pages)	
Ting Hu, Rui Li, and Jinming Dong	174702
A first principle study for the adsorption and absorption of carbon atom and the CO dissociation on Ir(100) surface (8 pages)	
I. A. Erikat and B. A. Hamad	174703

(Continued)

Theoretical study of amino derivatives and anticancer platinum drug grafted on various carbon nanostructures (11 pages)	S. Kraszewski, E. Duverger, C. Ramseyer, and F. Picaud	174704
Phase separation in antisymmetric films: A molecular dynamics study (6 pages)	Raishma Krishnan, Prabhat K. Jaiswal, and Sanjay Puri	174705
Effect of confinement on the solid-liquid coexistence of Lennard-Jones Fluid (13 pages)	Chandan K. Das and Jayant K. Singh	174706
Water dissociation on Ni(100) and Ni(111): Effect of surface temperature on reactivity (8 pages)	H. Seenivasan and Ashwani K. Tiwari	174707
Effective slippage on superhydrophobic trapezoidal grooves (11 pages)	Jiajia Zhou, Evgeny S. Asmolov, Friederike Schmid, and Olga I. Vinogradova	174708
Structure formation in perfluoropentacene:diindenoperylene blends and its impact on transient effects in the optical properties studied in real-time during growth (7 pages)	K. Broch, A. Gerlach, C. Lorch, J. Dieterle, J. Novák, A. Hinderhofer, and F. Schreiber	174709
Phononic crystals of spherical particles: A tight binding approach (11 pages)	M. Mattarelli, M. Secchi, and M. Montagna	174710
Favorable adsorption of capped amino acids on graphene substrate driven by desolvation effect (6 pages)	N. Dragneva, W. B. Floriano, D. Stauffer, R. C. Mawhinney, G. Fanchini, and O. Rubel	174711
Thermal transpiration through single walled carbon nanotubes and graphene channels (9 pages)	Joe Francis Thekkethala and Sarith P. Sathian	174712

Polymers and Soft Matter

Droplet size distributions in turbulent emulsions: Breakup criteria and surfactant effects from direct numerical simulations (14 pages)	R. Skartlien, E. Sollum, and H. Schumann	174901
Phase diagrams of Janus fluids with up-down constrained orientations (9 pages)	Riccardo Fantoni, Achille Giacometti, Miguel Ángel G. Maestre, and Andrés Santos	174902
Impurity effects on polaron-exciton formation in conjugated polymers (6 pages)	Luiz Antonio Ribeiro, Jr., Wiliam Ferreira da Cunha, Pedro Henrique de Oliveira Neto, Ricardo Gargano, and Geraldo Magela e Silva	174903
An atomistic description of the high-field degradation of dielectric polyethylene (9 pages)	Clive R. Bealing and R. Ramprasad	174904
Dynamics of polymer adsorption from dilute solution in shear flow near a planar wall (8 pages)	Sarit Dutta, Kevin D. Dorfman, and Satish Kumar	174905
Theory of polymer-dispersed cholesteric liquid crystals (10 pages)	Akihiko Matsuyama	174906

Biological Molecules and Networks

Dynamic neutron scattering from conformational dynamics. I. Theory and Markov models (10 pages)	Benjamin Lindner, Zheng Yi, Jan-Hendrik Prinz, Jeremy C. Smith, and Frank Noé	175101
Dynamic neutron scattering from conformational dynamics. II. Application using molecular dynamics simulation and Markov modeling (11 pages)	Zheng Yi, Benjamin Lindner, Jan-Hendrik Prinz, Frank Noé, and Jeremy C. Smith	175102

Vibrational spectroscopy of water in hydrated lipid multi-bilayers. III. Water clustering and vibrational energy transfer (10 pages)	
S. M. Gruenbaum and J. L. Skinner	175103
Stochastic dynamics of small ensembles of non-processive molecular motors: The parallel cluster model (27 pages)	
Thorsten Erdmann, Philipp J. Albert, and Ulrich S. Schwarz	175104

LETTERS TO THE EDITOR

Notes

Note: Evidence against 2D-Ising criticality in aqueous solutions with added salt (2 pages)	
Jacobo Troncoso and Claudio A. Cerdeiriña	176101

Errata

Publisher's Note: "Electron affinities and ionisation potentials for atoms via 'benchmark' tdDFT calculations with and without exchange kernels" [J. Chem. Phys. 138, 014109 (2013)] (1 page)	
Tim Gould and John F. Dobson	179901