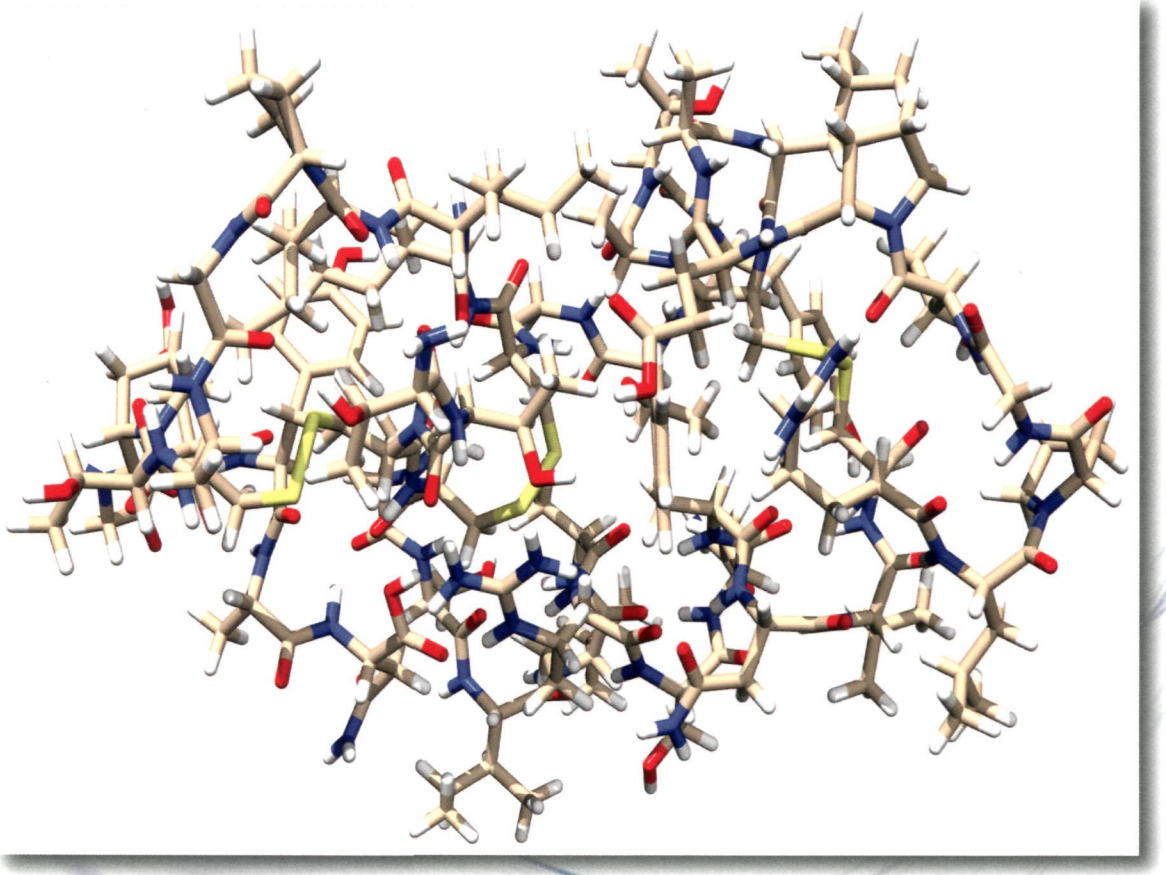
7 October 2013 Volume 139 Number 13

ПИ
J80/cp

AIP | The Journal of Chemical Physics



80th Anniversary

jcp.aip.org

THE JOURNAL OF CHEMICAL PHYSICS

Vol. 139, No. 13, 7 October 2013

CODEN: JCPSA6
ISSN: 0021-9606

▶ **Cover image** *from Christoph Riplinger, Barbara Sandhoefer, Andreas Hansen, and Frank Neese, J. Chem. Phys.* **139**, *134101 (2013).*

ARTICLES

Theoretical Methods and Algorithms

Natural triple excitations in local coupled cluster calculations with pair natural orbitals *(13 pages)*
Christoph Riplinger, Barbara Sandhoefer, Andreas Hansen, and Frank Neese **134101**

On the large interelectronic distance behavior of the correlation factor for explicitly correlated wave functions *(16 pages)*
Michał Lesiuk, Bogumił Jeziorski, and Robert Moszynski **134102**

The multi-layer multi-configuration time-dependent Hartree method for bosons: Theory, implementation, and applications *(19 pages)*
Lushuai Cao, Sven Krönke, Oriol Vendrell, and Peter Schmelcher **134103**

Time-resolved photoelectron imaging spectra from non-adiabatic molecular dynamics simulations *(9 pages)*
Alexander Humeniuk, Matthias Wohlgemuth, Toshinori Suzuki, and Roland Mitrić **134104**

General implementation of the resolution-of-the-identity and Cholesky representations of electron repulsion integrals within coupled-cluster and equation-of-motion methods: Theory and benchmarks *(16 pages)*
Evgeny Epifanovsky, Dmitry Zuev, Xintian Feng, Kirill Khistyaev, Yihan Shao, and Anna I. Krylov **134105**

A hybrid stochastic hierarchy equations of motion approach to treat the low temperature dynamics of non-Markovian open quantum systems *(9 pages)*
Jeremy M. Moix and Jianshu Cao **134106**

Heterogeneous nucleation in multi-component vapor on a partially wettable charged conducting particle. I. Formulation of general equations: Electrical surface and line excess quantities *(17 pages)*
M. Noppel, H. Vehkamäki, P. M. Winkler, M. Kulmala, and P. E. Wagner **134107**

Heterogeneous nucleation in multi-component vapor on a partially wettable charged conducting particle. II. The generalized Laplace, Gibbs-Kelvin, and Young equations and application to nucleation *(17 pages)*
M. Noppel, H. Vehkamäki, P. M. Winkler, M. Kulmala, and P. E. Wagner **134108**

A unifying mode-coupling theory for transport properties of electrolyte solutions. I. General scheme and limiting laws *(18 pages)*
Claudio Contreras Aburto and Gerhard Nägele **134109**

A unifying mode-coupling theory for transport properties of electrolyte solutions. II. Results for equal-sized ions electrolytes *(21 pages)*
Claudio Contreras Aburto and Gerhard Nägele **134110**

Efficiency at maximum power of a chemical engine *(8 pages)*
Hans Hooyberghs, Bart Cleuren, Alberto Salazar, Joseph O. Indekeu, and Christian Van den Broeck **134111**

Solution of the Dirac Coulomb equation for helium-like ions in the Poet-Temkin model *(8 pages)*
Li-Yan Tang, Yong-Bo Tang, Ting-Yun Shi, and J. Mitroy **134112**

(Continued)

Федеральное государственное бюджетное учреждение науки Центральная научная библиотека Уральского отделения Российской академии наук (ЦНБ УрО РАН)

© 2013 AIP Publishing LLC

Alternative separation of exchange and correlation energies in multi-configuration range-separated density-functional theory *(16 pages)*
Alexandrina Stoyanova, Andrew M. Teale, Julien Toulouse, Trygve Helgaker, and Emmanuel Fromager **134113**

Solving the Schroedinger equation using Smolyak interpolants *(14 pages)*
Gustavo Avila and Tucker Carrington, Jr. **134114**

Two-component Kramers restricted complete active space self-consistent field method with relativistic effective core potential *revisited*: Theory, implementation, and applications to spin-orbit splitting of lower *p*-block atoms *(14 pages)*
Inkoo Kim and Yoon Sup Lee **134115**

Advanced Experimental Techniques

High-precision drop shape analysis on inclining flat surfaces: Introduction and comparison of this special method with commercial contact angle analysis *(10 pages)*
Michael Schmitt and Florian Heib **134201**

Atoms, Molecules, and Clusters

Exploring the dynamics of C/H and C/Cl exchanges in the $C(^3P) + C_2H_3Cl$ reaction *(9 pages)*
Shih-Huang Lee, Wei-Kan Chen, Chih-Hao Chin, and Wen-Jian Huang **134301**

Dissociation of chloromethanes upon resonant σ^* excitation studied by x-ray scattering *(11 pages)*
R. Bohinc, M. Žitnik, K. Bučar, M. Kavčič, L. Journel, R. Guillemin, T. Marchenko, M. Simon, and W. Cao **134302**

The molecular structure of and interconversion tunneling in the argon-*cis*-1,2-difluoroethylene complex *(8 pages)*
Helen O. Leung, Mark D. Marshall, Jessica L. Mueller, and Brent K. Amberger **134303**

High-resolution infrared spectroscopy of atomic bromine in solid parahydrogen and orthodeuterium *(10 pages)*
Paul L. Raston, Sharon C. Kettwich, and David T. Anderson **134304**

Infrared-active spin-orbit transitions of halogen atom dopants in solid parahydrogen: The role of trapping site geometry *(10 pages)*
Robert J. Hinde **134305**

Selective coherent control of the lifetime of a resonance state with laser pulses *(9 pages)*
A. García-Vela **134306**

New analytical model for the ozone electronic ground state potential surface and accurate *ab initio* vibrational predictions at high energy range *(22 pages)*
Vladimir G. Tyuterev, Roman V. Kochanov, Sergey A. Tashkun, Filip Holka, and Péter G. Szalay **134307**

Liquids, Glasses, and Crystals

Tetratic phase of Hertzian spheres: Monte Carlo simulation *(5 pages)*
Takamichi Terao **134501**

Fundamental measure density functional theory study of liquid-vapor interface of dipolar and quadrupolar fluids *(8 pages)*
V. B. Warshavsky and X. C. Zeng **134502**

(Continued)

Broadband dynamics in neat 4-methyl-3-heptanol and in mixtures with 2-ethyl-1-hexanol *(10 pages)*
S. Bauer, H. Wittkamp, S. Schildmann, M. Frey, W. Hiller, T. Hecksher, N. B. Olsen, C. Gainaru, and R. Böhmer 134503

Secondary relaxations in a series of organic phosphate glasses revealed by dielectric spectroscopy *(7 pages)*
R. Kahlau, T. Dörfler, and E. A. Rössler 134504

Quantum molecular dynamics simulations of the thermophysical properties of shocked liquid ammonia for pressures up to 1.3 TPa *(7 pages)*
Dafang Li, Ping Zhang, and Jun Yan 134505

Structural motifs of pre-nucleation clusters *(8 pages)*
Y. Zhang, I. R. Türkmen, B. Wassermann, A. Erko, and E. Rühl 134506

Diffusivity and hydration of hydrazine in liquid and supercritical water through molecular dynamics simulations and split-flow pulse injection experiments *(7 pages)*
Dimitrios T. Kallikragas, Kashif I. Choudhry, Andriy Y. Plugatyr, and Igor M. Svishchev 134507

Surfaces, Interfaces, and Materials

A steady-state non-equilibrium molecular dynamics approach for the study of evaporation processes *(10 pages)*
Jianguo Zhang, Florian Müller-Plathe, Méziane Yahia-Ouahmed, and Frédéric Leroy 134701

Disordering and grain boundaries of $(Ni,Fe)Cr_2O_4$ spinels from atomistic calculations *(9 pages)*
Alain Chartier, Bogdan Golovchuk, Stéphane Gossé, and Laurent Van Brutzel 134702

Thermodynamics of extensive interfaces between rigid, apolar walls and water *(4 pages)*
E. S. Machlin 134703

Polymers and Soft Matter

Branching points in the low-temperature dipolar hard sphere fluid *(9 pages)*
Lorenzo Rovigatti, Sofia Kantorovich, Alexey O. Ivanov, José Maria Tavares, and Francesco Sciortino 134901

Molecular field theory for biaxial smectic A liquid crystals *(13 pages)*
T. B. T. To, T. J. Sluckin, and G. R. Luckhurst 134902

Polymerization-induced spinodal decomposition of ethylene glycol/phenolic resin solutions under electric fields *(8 pages)*
Gang Zhang and Guanjun Qiao 134903

Phase field method for nonequilibrium dynamics of reversible self-assembly systems *(6 pages)*
Karl F. Freed 134904

Effect of binding to carbon black on the dynamics of 1,4-polybutadiene *(7 pages)*
J. H. Roh, M. Tyagi, T. E. Hogan, and C. M. Roland 134905

One-dimensional potential of mean force underestimates activation barrier for transport across flexible lipid membranes *(12 pages)*
Dmitry I. Kopelevich 134906

Dynamics of edge dislocations in a sheared lamellar mesophase *(13 pages)*
V. Kumaran 134907

Zigzag transitions and nonequilibrium pattern formation in colloidal chains *(14 pages)*
Arthur V. Straube, Roel P. A. Dullens, Lutz Schimansky-Geier, and Ard A. Louis 134908

(Continued)

Size and boundary effects on the diffusive behavior of elongated colloidal particles in a strongly confined dense dispersion *(10 pages)*
Saber Naderi and Paul van der Schoot 134909

Numerical evidences for a free energy barrier in starlike polymer brushes *(8 pages)*
Wei Cui, Chan-Fei Su, Chen-Xu Wu, Holger Merlitz, and Jens-Uwe Sommer 134910

Biological Molecules and Networks

Optimization of collective enzyme activity via spatial localization *(11 pages)*
Alexander Buchner, Filipe Tostevin, Florian Hinzpeter, and Ulrich Gerland 135101

LETTERS TO THE EDITOR

Comments

Comment on "Temperature divergence of the dynamics of a poly(vinyl acetate) glass: Dielectric vs. mechanical behaviors" [J. Chem. Phys. 136, 154901 (2012)] *(2 pages)*
Ranko Richert 137101

Response to "Comment on 'Temperature divergence of the dynamics of a poly(vinyl acetate) glass: Dielectric vs. mechanical behaviors'" [J. Chem. Phys. 139, 137101 (2013)] *(2 pages)*
Jing Zhao and Gregory B. McKenna 137102

Errata

Publisher's Note: "Catch bond-like kinetics of helix cracking: Network analysis by molecular dynamics and Milestoning" [J. Chem. Phys. 139, 121902 (2013)] *(1 page)*
Steven M. Kreuzer, Tess J. Moon, and Ron Elber 139901

Erratum: "Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: The vertical transition approximation" [J. Chem. Phys. 139, 114102 (2013)] *(1 page)*
Maira D'Alessandro, Massimiliano Aschi, Claudia Mazzuca, Antonio Palleschi, and Andrea Amadei 139902

A publication of AIP Publishing LLC, Suite 1NO1, 2 Huntington Quadrangle, Melville, NY 11747-4502