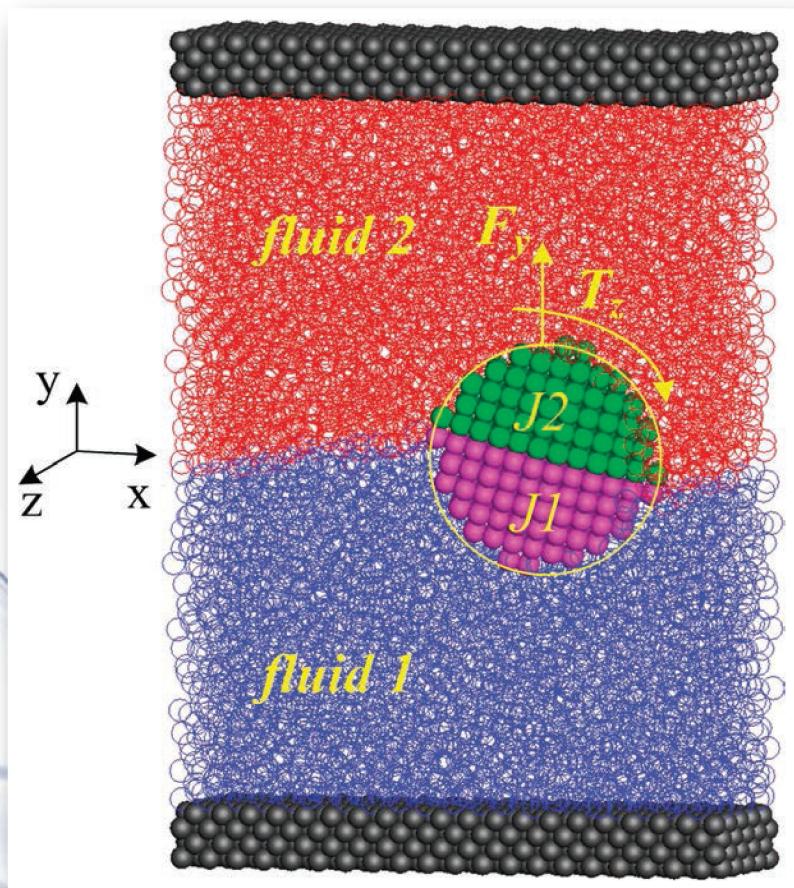


AIP | The Journal of Chemical Physics



FEATURED ARTICLE

Molecular simulation of translational and rotational diffusion of Janus nanoparticles at liquid interfaces EDITORIALS

Editorial: New editorial standards to better serve the community

Marsha L. Lester, Editor-in-Chief

J. Chem. Phys. **142**, 010401 (2015)

COMMUNICATIONS

Communication: Fast transport and relaxation of vibrational energy in polymer chains

Arkady A. Kurnosov, Igor V. Rubtsov and Alexander L. Burin

J. Chem. Phys. **142**, 011101 (2015);

Communication: Kinetics of scavenging of small, nucleating clusters: First nucleation theorem and sum rules

Jussi Malila, Robert McGraw, Ari Laaksonen and Kari E. J. Lehtinen

J. Chem. Phys. **142**, 011102 (2015);

ARTICLES

Theoretical Methods and Algorithms

Discontinuity of the exchange-correlation potential and the functional derivative of the noninteracting kinetic energy as the number of electrons crosses integer boundaries in Li, Be, and B

Robert C. Morrison

J. Chem. Phys. **142**, 014101 (2015)

On the convergence of perturbative coupled cluster triples expansions: Error cancellations in the CCSD(T) model and the importance of amplitude relaxation

Janus J. Eriksen, Poul Jorgensen and Jürgen Gauss

J. Chem. Phys. **142**, 014102 (2015)

Toward accurate thermochemistry of the ^{24}MgH , ^{25}MgH , and ^{26}MgH molecules at elevated temperatures: Corrections due to unbound states

Tamás Szidárovszky and Attila G. Császár

J. Chem. Phys. **142**, 014103 (2015)

An analysis of hydrated proton diffusion in ab initio molecular dynamics

Ying-Lung Steve Tse, Chris Knight and Gregory A. Voth

J. Chem. Phys. **142**, 014104 (2015)

Extracting the diffusion tensor from molecular dynamics simulation with Milestoning

Mauro L. Mugnai and Ron Elber

J. Chem. Phys. **142**, 014105 (2015);

Generalized method calculating the effective diffusion coefficient in periodic channels

Pavol Kalinay

J. Chem. Phys. **142**, 014106 (2015);

Accurate vibrational spectra via molecular tailoring approach: A case study of water clusters at MP2 level

Nityananda Sahu and Shridhar R. Gadre

J. Chem. Phys. **142**, 014107 (2015)

Advanced Experimental Techniques

Two-dimensional NMR measurement and point dipole model prediction of paramagnetic shift tensors in solids

Brennan J. Walder, Krishna K. Dey, Michael C. Davis, Jay H. Baltisberger and Philip J. Grandinetti

J. Chem. Phys. **142**, 014201 (2015);

Atoms, Molecules, and Clusters

Ultraviolet photodissociation action spectroscopy of the N-pyridinium cation

Christopher S. Hansen, Stephen J. Blanksby, Nahid Chalyavi, Evan J. Bieske, Jeffrey R. Reimers and Adam J. Trevitt

J. Chem. Phys. **142**, 014301 (2015); Planar dicyclic B_5S_6 , B_5S_6^- , and $\text{B}_5\text{S}_6^{2-}$ clusters: Boron sulfide analogues of naphthalene

Da-Zhi Li, Hui Bai, Ting Ou, Qiang Chen, Hua-Jin Zhai and Si-Dian Li

J. Chem. Phys. **142**, 014302 (2015)

Pressure effects on the relaxation of an excited nitromethane molecule in an argon bath

[Luis A. Rivera-Rivera](#), [Albert F. Wagner](#), [Thomas D. Sewell](#) and [Donald L. Thompson](#)

J. Chem. Phys. **142**, 014303 (2015);

Interaction of O⁻ and H₂ at low temperatures

[P. Jusko](#), [Š. Roučka](#), [D. Mulin](#), [I. Zymák](#), [R. Plašil](#), [D. Gerlich](#), [M. Čížek](#), [K. Houfek](#) and [J. Glosík](#)

J. Chem. Phys. **142**, 014304 (2015)

An experimental and theoretical study of the electronic spectrum of the HBCl free radical

[Mohammed A. Gharabeih](#), [Ramya Nagarajan](#), [Dennis J. Clouthier](#) and [Riccardo Tarroni](#)

J. Chem. Phys. **142**, 014305 (2015)

Rotationally inelastic scattering of methyl radicals with Ar and N₂

[Ondřej Tkáč](#), [Qianli Ma](#) (马千里), [Martin Stej](#), [Andrew J. Orr-Ewing](#) and [Paul J. Dagdigian](#)

J. Chem. Phys. **142**, 014306 (2015)

Single photon simultaneous K-shell ionization and K-shell excitation. I. Theoretical model applied to the interpretation of experimental results on H₂O

[S. Carniato](#), [P. Selles](#), [L. Andrić](#), [J. Palaudoux](#), [F. Penent](#), [M. Žitník](#), [K. Bučar](#), [M. Nakano](#), [Y. Hikosaka](#), [K. Ito](#) and [P. Lablanquie](#)

J. Chem. Phys. **142**, 014307 (2015);

Single photon simultaneous K-shell ionization and K-shell excitation. II. Specificities of hollow nitrogen molecular ions

[S. Carniato](#), [P. Selles](#), [L. Andrić](#), [J. Palaudoux](#), [F. Penent](#), [M. Žitník](#), [K. Bučar](#), [M. Nakano](#), [Y. Hikosaka](#), [K. Ito](#) and [P. Lablanquie](#)

J. Chem. Phys. **142**, 014308 (2015);

Quantum dynamics study on the CHIPR potential energy surface for the hydroperoxy radical: The reactions O + OH ⇌ O₂ + H

[Marc Moix Teixidor](#) and [António J. C. Varandas](#)

J. Chem. Phys. **142**, 014309 (2015)

Vibrational predissociation and vibrationally induced isomerization of 3-amino phenol-ammonia

[Cornelia G. Heid](#), [Wyatt G. Merrill](#), [Amanda S. Case](#) and [F. Fleming Crim](#)

J. Chem. Phys. **142**, 014310 (2015)

Helium induced fine structure in the electronic spectra of anthracene derivatives doped into superfluid helium nanodroplets

[D. Pentlehner](#) and [A. Slenczka](#)

J. Chem. Phys. **142**, 014311 (2015);

Liquids, Glasses, and Crystals

Dopant effects on 2-ethyl-1-hexanol: A dual-channel impedance spectroscopy and neutron scattering study

[Lokendra P. Singh](#), [Ahmed Raihane](#), [Christiane Alba-Simionescu](#) and [Ranko Richert](#)

J. Chem. Phys. **142**, 014501 (2015)

Conformation and interactions of dopamine hydrochloride in solution

[Samantha K. Callear](#), [Andrew Johnston](#), [Sylvia E. McLain](#) and [Silvia Imberti](#)

J. Chem. Phys. **142**, 014502 (2015)

Study of the thermodynamic properties of CeO₂ from ab initio calculations: The effect of phonon-phonon interaction

[Zhen-Wei Niu](#), [Zhao-Yi Zeng](#), [Cui-E Hu](#), [Ling-Cang Cai](#) and [Xiang-Rong Chen](#)

J. Chem. Phys. **142**, 014503 (2015)

Sensing polarization effects through the analysis of the effective C₆ dispersion coefficients in NaCl solutions

[Alfredo Guevara-García](#), [Joel Ireta](#) and [Marcelo Galván](#)

J. Chem. Phys. **142**, 014504 (2015)

In silico infrared and Raman spectroscopy under pressure: The case of CaSnO₃ perovskite

[J. Maul](#), [A. Erba](#), [L. M. G. Santos](#), [J. R. Sambrano](#) and [R. Dovesi](#)

J. Chem. Phys. **142**, 014505 (2015);

A structural study of a two-dimensional electrolyte by Monte Carlo simulations

[Jana Aupic](#) and [Tomaz Urbic](#)

J. Chem. Phys. **142**, 014506 (2015);

Surfaces, Interfaces, and Materials

Molecular simulation of translational and rotational diffusion of Janus nanoparticles at liquid interfaces

[Hossein Rezvantalab](#), [German Drazer](#) and [Shahab Shojaei-Zadeh](#)

J. Chem. Phys. **142**, 014701 (2015);

Demixing and confinement of non-additive hard-sphere mixtures in slit pores

[N. G. Almarza](#), [C. Martín](#), [E. Lomba](#) and [C. Bores](#)

J. Chem. Phys. **142**, 014702 (2015);

Investigation of the deposition and thermal behavior of striped phases of unsymmetric disulfide self-assembled monolayers on Au(111): The case of 11-hydroxyundecyl decyl disulfide

[Erol Albayrak](#), [Semistan Karabuga](#), [Gianangelo Bracco](#) and [M. Fatih Danışman](#)

J. Chem. Phys. **142**, 014703 (2015);

Modeling selective intergranular oxidation of binary alloys

[Zhijie Xu](#), [Dongsheng Li](#), [Daniel K. Schreiber](#), [Kevin M. Rosso](#) and [Stephen M. Bruemmer](#)

J. Chem. Phys. **142**, 014704 (2015);

Contact theorems for anisotropic fluids near a hard wall

[M. Holovko](#) and [D. di Caprio](#)

J. Chem. Phys. **142**, 014705 (2015);

Polymers and Soft Matter

Probing the molecular connectivity of water confined in polymer hydrogels

[B. Rossi](#), [V. Venuti](#), [A. Mele](#), [C. Punta](#), [L. Melone](#), [V. Crupi](#), [D. Majolino](#), [F. Trotta](#), [F. D'Amico](#), [A. Gessini](#) and [C. Masciovecchio](#)
J. Chem. Phys. **142**, 014901 (2015);

Virial coefficients and demixing in the Asakura–Oosawa model

[Mariano López de Haro](#), [Carlos F. Tejero](#), [Andrés Santos](#), [Santos B. Yuste](#), [Giacomo Fiumara](#) and [Franz Sajja](#)
J. Chem. Phys. **142**, 014902 (2015);

Bistability in a self-assembling system confined by elastic walls: Exact results in a one-dimensional lattice model

[J. Pekalski](#), [A. Ciech](#) and [N. G. Almarza](#)
J. Chem. Phys. **142**, 014903 (2015);

Hydrodynamic interactions between a sphere and a number of small particles

[Maria L. Ekiel-Jeżewska](#) and [B. U. Felderhof](#)
J. Chem. Phys. **142**, 014904 (2015);

The meaning of the “universal” WLF parameters of glass-forming polymer liquids

[Jacek Dudowicz](#), [Jack F. Douglas](#) and [Karl F. Freed](#)
J. Chem. Phys. **142**, 014905 (2015);

Chain end mobilities in polymer melts—A computational study

[Diddo Diddens](#) and [Andreas Heuer](#)

J. Chem. Phys. **142**, 014906 (2015);

Biological Molecules and Networks

Effect of temperature on the low-frequency vibrational spectrum and relative structuring of hydration water around a single-stranded DNA
[Kaushik Chakraborty](#) and [Sanjoy Bandyopadhyay](#)
J. Chem. Phys. **142**, 015101 (2015);

Biological Molecules and Networks

The effects of multiple probes on the hybridization of target DNA on surfaces
Ryan C. Welling and Thomas A. Knotts IV
J. Chem. Phys. **142**, 015102 (2015);
Kinetic regulation mechanism of pbuE riboswitch
Sha Gong, Yujie Wang and Wenbing Zhang
J. Chem. Phys. **142**, 015103 (2015);

LETTERS TO THE EDITOR

Errata

Erratum: “Third and fourth virial coefficients for hard disks in narrow channels” [J. Chem. Phys. **140, 244504 (2014)]**
K. K. Mon
J. Chem. Phys. **142**, 019901 (2015);