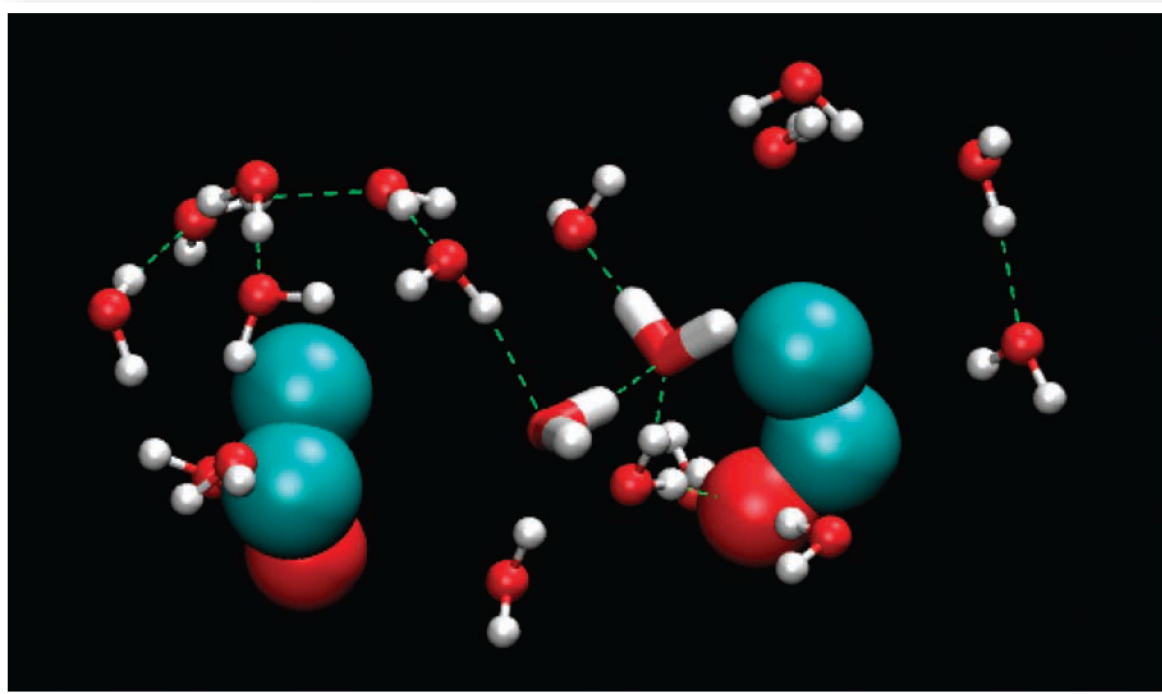


14 February 2015

Volume 142 Number 6

AIP | The Journal of Chemical Physics



jcp.aip.org

COMMUNICATIONS

Communication: Surface-to-bulk diffusion of isolated versus interacting C atoms in Ni(111) and Cu(111) substrates: A first principle investigation

Abhilash Harpale, Marco Panesi and Huck Beng Chew

J. Chem. Phys. **142**, 061101 (2015); <http://dx.doi.org/10.1063/1.4907716>

ARTICLES

Theoretical Methods and Algorithms

Stochastic linear multistep methods for the simulation of chemical kinetics

Manuel Barrio, Kevin Burrage and Pamela Burrage

J. Chem. Phys. **142**, 064101 (2015); <http://dx.doi.org/10.1063/1.4907008>

Does DFT-SAPT method provide spectroscopic accuracy?

Leonid Shirkov and Jan Makarewicz

J. Chem. Phys. **142**, 064102 (2015); <http://dx.doi.org/10.1063/1.4907204>

Caveats of mean first-passage time methods applied to the crystallization transition: Effects of non-Markovianity

Svetlana Jungblut and Christoph Dellago

J. Chem. Phys. **142**, 064103 (2015); <http://dx.doi.org/10.1063/1.4907364>

Bloch-Redfield equations for modeling light-harvesting complexes

Jan Jeske, David J. Ing, Martin B. Plenio, Susana F. Huelga and Jared H. Cole

J. Chem. Phys. **142**, 064104 (2015); <http://dx.doi.org/10.1063/1.4907370>

On the covariant description of diffusion in two-dimensional confined environments

Angel A. García-Chung, Guillermo Chacón-Acosta and Leonardo Dagdug

J. Chem. Phys. **142**, 064105 (2015); <http://dx.doi.org/10.1063/1.4907553>

Model space diabaticization for quantum photochemistry

Shaohong L. Li, Donald G. Truhlar, Michael W. Schmidt and Mark S. Gordon

J. Chem. Phys. **142**, 064106 (2015); <http://dx.doi.org/10.1063/1.4907038>

The charge-asymmetric nonlocally determined local-electric (CANDLE) solvation model

Ravishankar Sundararaman and William A. Goddard III

J. Chem. Phys. **142**, 064107 (2015); <http://dx.doi.org/10.1063/1.4907731>

Non-orthogonal spin-adaptation of coupled cluster methods: A new implementation of methods including quadruple excitations

Devin A. Matthews and John F. Stanton

J. Chem. Phys. **142**, 064108 (2015); <http://dx.doi.org/10.1063/1.4907278>

Analytic derivative couplings in time-dependent density functional theory: Quadratic response theory versus pseudo-wavefunction approach

Xing Zhang and John M. Herbert

J. Chem. Phys. **142**, 064109 (2015); <http://dx.doi.org/10.1063/1.4907376>

Correlated electron pseudopotentials for 3d-transition metals

J. R. Trail and R. J. Needs

J. Chem. Phys. **142**, 064110 (2015); <http://dx.doi.org/10.1063/1.4907589>

Accurate thermochemistry from explicitly correlated distinguishable cluster approximation

Daniel Kats, David Kreplin, Hans-Joachim Werner and Frederick R. Manby

J. Chem. Phys. **142**, 064111 (2015); <http://dx.doi.org/10.1063/1.4907591>

Fermi orbital derivatives in self-interaction corrected density functional theory: Applications to closed shell atoms

Mark R. Pederson

J. Chem. Phys. **142**, 064112 (2015); <http://dx.doi.org/10.1063/1.4907592>

Order and disorder in irreversible decay processes

Jonathan W. Nichols, Shane W. Flynn and Jason R. Green

J. Chem. Phys. **142**, 064113 (2015); <http://dx.doi.org/10.1063/1.4907629>

First-order derivative couplings between excited states from adiabatic TDDFT response theory

Qi Ou, Gregory D. Bellchambers, Filipp Furche and Joseph E. Subotnik

J. Chem. Phys. **142**, 064114 (2015); <http://dx.doi.org/10.1063/1.4906941>

Statistical mechanics of Hamiltonian adaptive resolution simulations

P. Español, R. Delgado-Buscalioni, R. Everaers, R. Potestio, D. Donadio and K. Kremer

J. Chem. Phys. **142**, 064115 (2015); <http://dx.doi.org/10.1063/1.4907006>

Accuracy of buffered-force QM/MM simulations of silica

Anke Peguiron, Lucio Colombi Ciacchi, Alessandro De Vita, James R. Kermode and Gianpietro Moras

J. Chem. Phys. **142**, 064116 (2015); <http://dx.doi.org/10.1063/1.4907786>

Maximum probability domains for the analysis of the microscopic structure of liquids

Federica Agostini, Giovanni Ciccotti, Andreas Savin and Rodolphe Vuilleumier

J. Chem. Phys. **142**, 064117 (2015); <http://dx.doi.org/10.1063/1.4907406>

Two-photon absorption cross sections within equation-of-motion coupled-cluster formalism using resolution-of-the-identity and Cholesky decomposition representations: Theory, implementation, and benchmarks

Kaushik D. Nanda and Anna I. Krylov

J. Chem. Phys. **142**, 064118 (2015); <http://dx.doi.org/10.1063/1.4907715>

Advanced Experimental Techniques

Cross-polarization phenomena in the NMR of fast spinning solids subject to adiabatic sweeps

Sungsool Wi, Zhehong Gan, Robert Schurko and Lucio Frydman

J. Chem. Phys. **142**, 064201 (2015); <http://dx.doi.org/10.1063/1.4907206>

Atoms, Molecules, and Clusters

Alkali metal mediated C–C bond coupling reaction

Hiroto Tachikawa

J. Chem. Phys. **142**, 064301 (2015); <http://dx.doi.org/10.1063/1.4906944>

An auxiliary-field quantum Monte Carlo study of the chromium dimer

Wirawan Purwanto, Shiwei Zhang and Henry Krakauer

J. Chem. Phys. **142**, 064302 (2015); <http://dx.doi.org/10.1063/1.4906829>

Electronic excitation of carbonyl sulphide (COS) by high-resolution vacuum ultraviolet photoabsorption and electron-impact spectroscopy in the energy region from 4 to 11 eV

P. Limão-Vieira, F. Ferreira da Silva, D. Almeida, M. Hoshino, H. Tanaka, D. Mogi, T. Tanioka, N. J. Mason, S. V. Hoffmann, M.-J. Hubin-Franskin and J. Delwiche

J. Chem. Phys. **142**, 064303 (2015); <http://dx.doi.org/10.1063/1.4907200>

Lithium formate ion clusters formation during electrospray ionization: Evidence of magic number clusters by mass spectrometry and ab initio calculations

Anil Shukla and Bogdan Bogdanov

J. Chem. Phys. **142**, 064304 (2015); <http://dx.doi.org/10.1063/1.4907366>

Photoelectron spectra of CeO⁻ and Ce(OH)₂⁻

Manisha Ray, Jeremy A. Felton, Jared O. Kafader, Josey E. Topolski and Caroline Chick Jarrold

J. Chem. Phys. **142**, 064305 (2015); <http://dx.doi.org/10.1063/1.4907714>

Comparison of the local binding motifs in the imidazolium-based ionic liquids [EMIM][BF₄] and [EMMIM][BF₄] through cryogenic ion vibrational predissociation spectroscopy: Unraveling the roles of anharmonicity and intermolecular interactions

Joseph A. Fournier, Conrad T. Wolke, Christopher J. Johnson, Anne B. McCoy and Mark A. Johnson

J. Chem. Phys. **142**, 064306 (2015); <http://dx.doi.org/10.1063/1.4907199>

Ab initio dynamics of the cytochrome P450 hydroxylation reaction

Justin E. Elenewski and John C Hackett

J. Chem. Phys. **142**, 064307 (2015); <http://dx.doi.org/10.1063/1.4907733>

State-to-state reaction dynamics of $^{18}\text{O}+^{32}\text{O}_2$ studied by a time-dependent quantum wavepacket method

Wenbo Xie, Lan Liu, Zhigang Sun, Hua Guo and Richard Dawes

J. Chem. Phys. **142**, 064308 (2015); <http://dx.doi.org/10.1063/1.4907229>

Full-dimensional and reduced-dimensional calculations of initial state-selected reaction probabilities studying the $\text{H} + \text{CH}_4 \rightarrow \text{H}_2 + \text{CH}_3$ reaction on a neural network PES

Ralph Welsch and Uwe Manthe

J. Chem. Phys. **142**, 064309 (2015); <http://dx.doi.org/10.1063/1.4906825>

The fundamental rotational interval of para- H_2 by MQDT-assisted Rydberg spectroscopy of H_2

Christa Haase, Maximilian Beyer, Christian Jungen and Frédéric Merkt

J. Chem. Phys. **142**, 064310 (2015); <http://dx.doi.org/10.1063/1.4907531>

Relativistic effects for the reaction $\text{Sg} + 6 \text{CO} \rightarrow \text{Sg}(\text{CO})_6$: Prediction of the mean bond energy, atomization energy, and existence of the first organometallic transactinide superheavy hexacarbonyl $\text{Sg}(\text{CO})_6$

Gulzari L. Malli

J. Chem. Phys. **142**, 064311 (2015); <http://dx.doi.org/10.1063/1.4907595>

Experimental and theoretical investigation of the first-order hyperpolarizability of a class of triarylamine derivatives

Daniel L. Silva, Ruben D. Fonseca, Marcelo G. Vivas, E. Ishow, Sylvio Canuto, Cleber R. Mendonca and Leonardo De Boni

J. Chem. Phys. **142**, 064312 (2015); <http://dx.doi.org/10.1063/1.4906893>

Symmetry breaking and excitonic effects on optical properties of defective nanographenes

Yoshifumi Noguchi and Osamu Sugino

J. Chem. Phys. **142**, 064313 (2015); <http://dx.doi.org/10.1063/1.4907751>

A full-dimensional quantum dynamics study of the mode specificity in the $\text{H} + \text{HOD}$ abstraction reaction

Bina Fu and Dong H. Zhang

J. Chem. Phys. **142**, 064314 (2015); <http://dx.doi.org/10.1063/1.4907918>

A molecular symmetry analysis of the electronic states and transition dipole moments for molecules with two torsional degrees of freedom

R. Obaid and M. Leibscher

J. Chem. Phys. **142**, 064315 (2015); <http://dx.doi.org/10.1063/1.4907405>

Dissociative electron attachments to ethanol and acetaldehyde: A combined experimental and simulation study

Xu-Dong Wang, Chuan-Jin Xuan, Wen-Ling Feng and Shan Xi Tian

J. Chem. Phys. **142**, 064316 (2015); <http://dx.doi.org/10.1063/1.4907940>

Simultaneous analysis of the Ballik-Ramsay and Phillips systems of C_2 and observation of forbidden transitions between singlet and triplet states

Wang Chen, Kentarou Kawaguchi, Peter F. Bernath and Jian Tang

J. Chem. Phys. **142**, 064317 (2015); <http://dx.doi.org/10.1063/1.4907530>

Liquids, Glasses, and Crystals

Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures

Ming-Liang Tan, Benjamin T. Miller, Jerez Te, Joseph R. Cendagorta, Bernard R. Brooks and Toshiko Ichiye

J. Chem. Phys. **142**, 064501 (2015); <http://dx.doi.org/10.1063/1.4906750>

Evidence for weakly bound electrons in non-irradiated alkane crystals: The electrons as a probe of structural differences in crystals

M. Pietrow, M. Gagoś, L. E. Misiak, K. Kornarzyński, J. Szurkowski, P. Rochowski and M. Grzegorzcyk

J. Chem. Phys. **142**, 064502 (2015); <http://dx.doi.org/10.1063/1.4907262>

Effects of polarizability on the structural and thermodynamics properties of $[\text{C}_n\text{mim}][\text{Gly}]$ ionic liquids ($n = 1-4$) using EEM/MM molecular dynamic simulations

Yang Wu, Na Hu, Lili Yue, Lihong Wei and Wei Guan

J. Chem. Phys. **142**, 064503 (2015); <http://dx.doi.org/10.1063/1.4907281>

Dynamic correlation length scales under isochronal conditions

R. Casalini, D. Fragiadakis and C. M. Roland

J. Chem. Phys. **142**, 064504 (2015); <http://dx.doi.org/10.1063/1.4907371>

Nonlinear ion transport in the supercooled ionic liquid 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide: Frequency dependence of third-order and fifth-order conductivity coefficients

L. N. Patro, O. Burghaus and B. Roling

J. Chem. Phys. **142**, 064505 (2015); <http://dx.doi.org/10.1063/1.4907373>

Nuclear quantum effects on the high pressure melting of dense lithium

Yexin Feng, Ji Chen, Dario Alfè, Xin-Zheng Li and Enge Wang
J. Chem. Phys. **142**, 064506 (2015); <http://dx.doi.org/10.1063/1.4907752>

The relationship between reorientational molecular motions and phase transitions in [Mg(H₂O)₆](BF₄)₂, studied with the use of ¹H and ¹⁹F NMR and FT-MIR

Edward Mikuli, Joanna Hetmańczyk, Bartłomiej Grad, Asja Kozak, Jan W. Wąsicki, Paweł Bilski, Krystyna Holderna-Natkaniec and Wojciech Medycki
J. Chem. Phys. **142**, 064507 (2015); <http://dx.doi.org/10.1063/1.4907372>

Structural evolution during fragile-to-strong transition in CuZr(Al) glass-forming liquids

Chao Zhou, Lina Hu, Qijing Sun, Haijiao Zheng, Chunzhi Zhang and Yuanzheng Yue
J. Chem. Phys. **142**, 064508 (2015); <http://dx.doi.org/10.1063/1.4907374>

Nuclear quantum effects in water exchange around lithium and fluoride ions

David M. Wilkins, David E. Manolopoulos and Liem X. Dang
J. Chem. Phys. **142**, 064509 (2015); <http://dx.doi.org/10.1063/1.4907554>

Interaction of ions, atoms, and small molecules with quantized vortex lines in superfluid ⁴He

David Mateo, Jussi Eloranta and Gary A. Williams
J. Chem. Phys. **142**, 064510 (2015); <http://dx.doi.org/10.1063/1.4907597>

Third order dielectric time dependent susceptibilities and the "box model"

R. M. Pick
J. Chem. Phys. **142**, 064511 (2015); <http://dx.doi.org/10.1063/1.4906807>

Extended Lagrangian Born-Oppenheimer molecular dynamics simulations of the shock-induced chemistry of phenylacetylene

M. J. Cawkwell, Anders M. N. Niklasson and Dana M. Dattelbaum
J. Chem. Phys. **142**, 064512 (2015); <http://dx.doi.org/10.1063/1.4907909>

Surfaces, Interfaces, and Materials

A scale-bridging modeling approach for anisotropic organic molecules at patterned semiconductor surfaces

Nicola Kleppmann and Sabine H. L. Klapp
J. Chem. Phys. **142**, 064701 (2015); <http://dx.doi.org/10.1063/1.4907037>

On the feasibility of silicene encapsulation by AlN deposited using an atomic layer deposition process

H. Van Bui, F. B. Wiggers, R. Friedlein, Y. Yamada-Takamura, A. Y. Kovalgin and M. P. de Jong
J. Chem. Phys. **142**, 064702 (2015); <http://dx.doi.org/10.1063/1.4907375>

Evaluation of finite-size effects in cavitation and droplet formation

Øivind Wilhelmsen and David Reguera
J. Chem. Phys. **142**, 064703 (2015); <http://dx.doi.org/10.1063/1.4907367>

Crystallization in supercooled liquid Cu: Homogeneous nucleation and growth

J. C. E. L. Wang, Y. Cai, H. A. Wu and S. N. Luo
J. Chem. Phys. **142**, 064704 (2015); <http://dx.doi.org/10.1063/1.4907627>

Ab initio atomistic thermodynamics study on the oxidation mechanism of binary and ternary alloy surfaces

Shi-Yu Liu, Shiyang Liu, De-Jun Li, Sanwu Wang, Jing Guo and Yaogen Shen
J. Chem. Phys. **142**, 064705 (2015); <http://dx.doi.org/10.1063/1.4907718>

Tolman length and rigidity constants of the Lennard-Jones fluid

Øivind Wilhelmsen, Dick Bedeaux and David Reguera
J. Chem. Phys. **142**, 064706 (2015); <http://dx.doi.org/10.1063/1.4907588>

Squeezout phenomena and boundary layer formation of a model ionic liquid under confinement and charging

R. Capozza, A. Vanossi, A. Benassi and E. Tosatti
J. Chem. Phys. **142**, 064707 (2015); <http://dx.doi.org/10.1063/1.4907747>

The growth of sulfur adlayers on Au(100)

Yue Jiang, Xihui Liang, Shendong Ren, Chi-Lu Chen, Liang-Jen Fan, Yaw-Wen Yang, Jian-Ming Tang and Dah-An Luh
J. Chem. Phys. **142**, 064708 (2015); <http://dx.doi.org/10.1063/1.4907789>

Polymers and Soft Matter

How the flow affects the phase behaviour and microstructure of polymer nanocomposites

Pavlos S. Stephanou

J. Chem. Phys. **142**, 064901 (2015); <http://dx.doi.org/10.1063/1.4907363>

Distribution of distances between DNA barcode labels in nanochannels close to the persistence length

Wesley F. Reinhart, Jeff G. Reifenberger, Damini Gupta, Abhiram Muralidhar, Julian Sheats, Han Cao and Kevin D. Dorfman

J. Chem. Phys. **142**, 064902 (2015); <http://dx.doi.org/10.1063/1.4907552>

Isotropic-nematic phase equilibria of hard-sphere chain fluids—Pure components and binary mixtures

Bernardo Oyarzún, Thijs van Westen and Thijs J. H. Vlugt

J. Chem. Phys. **142**, 064903 (2015); <http://dx.doi.org/10.1063/1.4907639>

Relaxation processes in a lower disorder order transition diblock copolymer

Alejandro Sanz, Tiberio A. Ezquerra, Rebeca Hernández, Michael Sprung and Aurora Nogales

J. Chem. Phys. **142**, 064904 (2015); <http://dx.doi.org/10.1063/1.4907722>

Short-time diffusion in concentrated bidisperse hard-sphere suspensions

Mu Wang, Marco Heinen and John F. Brady

J. Chem. Phys. **142**, 064905 (2015); <http://dx.doi.org/10.1063/1.4907594>

Biological Molecules and Networks

Asynchronous symmetry-based sequences for homonuclear dipolar recoupling in solid-state nuclear magnetic resonance

Kong Ooi Tan, M. Rajeswari, P. K. Madhu and Matthias Ernst

J. Chem. Phys. **142**, 065101 (2015); <http://dx.doi.org/10.1063/1.4907275>

LETTERS TO THE EDITOR

Errata

Erratum: “Restricted active space calculations of L-edge X-ray absorption spectra: From molecular orbitals to multiplet states” [J. Chem. Phys. 141, 124116 (2014)]

Rahul V. Pinjari, Mickaël G. Delcey, Meiyuan Guo, Michael Odelius and Marcus Lundberg

J. Chem. Phys. **142**, 069901 (2015); <http://dx.doi.org/10.1063/1.4908043>

Erratum: “Effect of the asymmetry of the coupling of the redox molecule to the electrodes in the one-level electrochemical bridged tunneling contact on the Coulomb blockade and the operation of molecular transistor” [J. Chem. Phys. 141, 124706 (2014)]

Igor G. Medvedev

J. Chem. Phys. **142**, 069902 (2015); <http://dx.doi.org/10.1063/1.4908233>