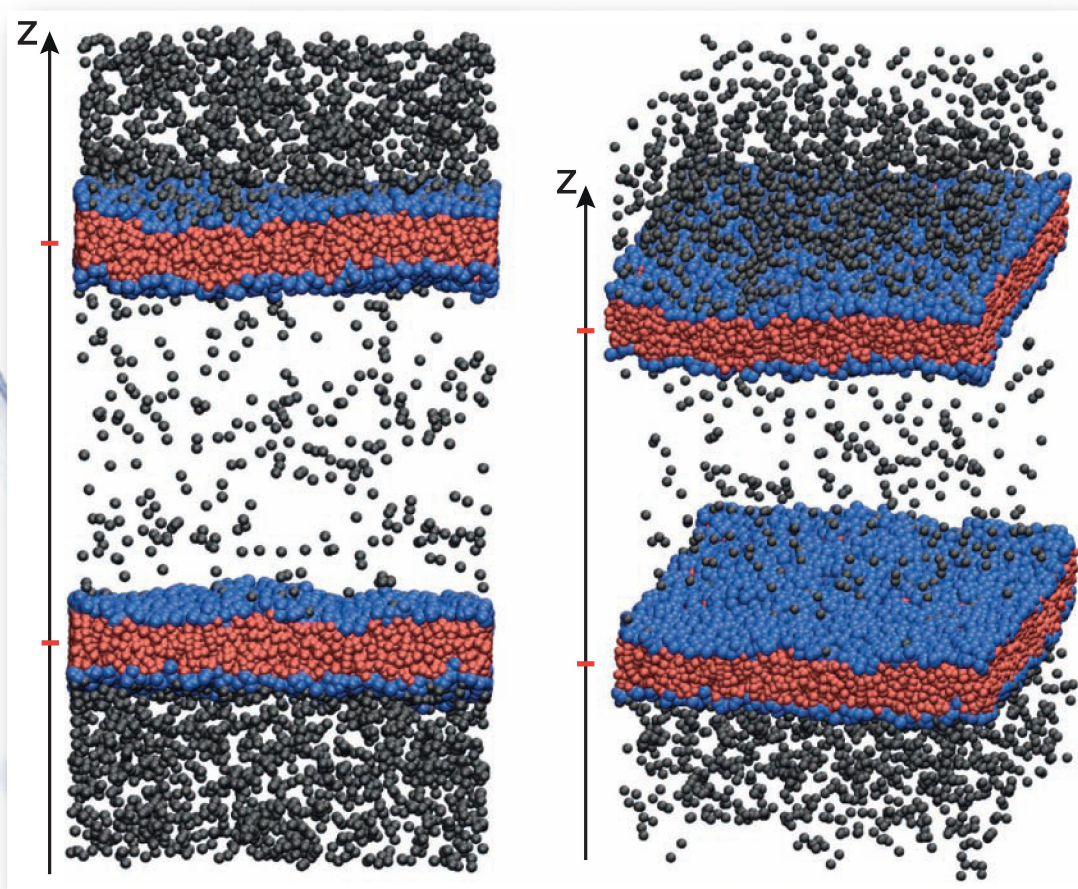


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COMMUNICATIONS

Communication: Evidence of stable van der Waals CO₂ clusters relevant to Venus atmosphere conditions

Ruslan E. Asfin, Jeanna V. Buldyreva, Tatyana N. Sinyakova, Daniil V. Oparin and Nikolai N. Filippov
J. Chem. Phys. **142**, 051101 (2015); <http://dx.doi.org/10.1063/1.4906874>

Communication: Satisfying fermionic statistics in the modeling of open time-dependent quantum systems with one-electron reduced density matrices

Kade Head-Marsden and David A. Mazziotti
J. Chem. Phys. **142**, 051102 (2015); <http://dx.doi.org/10.1063/1.4906942>

Communication: Automatic code generation enables nuclear gradient computations for fully internally contracted multireference theory

Matthew K. MacLeod and Toru Shiozaki
J. Chem. Phys. **142**, 051103 (2015); <http://dx.doi.org/10.1063/1.4907717>

Communication: Pair interaction ordering in fluids with random interactions

Lenin S. Shagolsem, Dino Osmanović, Orit Peleg and Yitzhak Rabin
J. Chem. Phys. **142**, 051104 (2015); <http://dx.doi.org/10.1063/1.4907730>

ARTICLES

Theoretical Methods and Algorithms

Spontaneous curvature of bilayer membranes from molecular simulations: Asymmetric lipid densities and asymmetric adsorption

Bartosz Różycki and Reinhard Lipowsky
J. Chem. Phys. **142**, 054101 (2015); <http://dx.doi.org/10.1063/1.4906149>

Spicing up continuum solvation models with SaLSA: The spherically averaged liquid susceptibility ansatz

Ravishankar Sundararaman, Kathleen A. Schwarz, Kendra Letchworth-Weaver and T. A. Arias
J. Chem. Phys. **142**, 054102 (2015); <http://dx.doi.org/10.1063/1.4906828>

Complex basis functions revisited: Implementation with applications to carbon tetrafluoride and aromatic N-containing heterocycles within the static-exchange approximation

Alec F. White, Martin Head-Gordon and C. William McCurdy
J. Chem. Phys. **142**, 054103 (2015); <http://dx.doi.org/10.1063/1.4906940>

Revisiting the chemical reactivity indices as the state function derivatives. The role of classical chemical hardness

Ali Malek and Robert Balawender
J. Chem. Phys. **142**, 054104 (2015); <http://dx.doi.org/10.1063/1.4906555>

Generalized gradient approximation exchange energy functional with correct asymptotic behavior of the corresponding potential

Javier Carmona-Espíndola, José L. Gázquez, Alberto Vela and S. B. Trickey
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J. Chem. Phys. **142**, 054106 (2015); <http://dx.doi.org/10.1063/1.4907269>

Origin of molecular conformational stability: Perspectives from molecular orbital interactions and density functional reactivity theory

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Bob Martin and Jochen Autschbach
J. Chem. Phys. **142**, 054108 (2015); <http://dx.doi.org/10.1063/1.4906318>

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J. Chem. Phys. **142**, 054201 (2015); <http://dx.doi.org/10.1063/1.4907277>

Atoms, Molecules, and Clusters

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Matthew D. Brynteson and Laurie J. Butler
J. Chem. Phys. **142**, 054301 (2015); <http://dx.doi.org/10.1063/1.4905776>

A comparison of neutral and charged species of one- and two-dimensional models of graphene nanoribbons using multireference theory

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J. Chem. Phys. **142**, 054302 (2015); <http://dx.doi.org/10.1063/1.4906540>

Peroxyacetyl radical: Electronic excitation energies, fundamental vibrational frequencies, and symmetry breaking in the first excited state

Andreas V. Copan, Avery E. Wiens, Ewa M. Nowara, Henry F. Schaefer III and Jay Agarwal
J. Chem. Phys. **142**, 054303 (2015); <http://dx.doi.org/10.1063/1.4906490>

Electronic structure, stability, and oxidation of boron-magnesium clusters and cluster solids

Arthur C. Reber and Shiv N. Khanna
J. Chem. Phys. **142**, 054304 (2015); <http://dx.doi.org/10.1063/1.4907273>

HXeI and HXeH in Ar, Kr, and Xe matrices: Experiment and simulation

Cheng Zhu, Keisuke Niimi, Tetsuya Taketsugu, Masashi Tsuge, Akira Nakayama and Leonid Khriachtchev
J. Chem. Phys. **142**, 054305 (2015); <http://dx.doi.org/10.1063/1.4906875>

The influence of oxygen adsorption on the NEXAFS and core-level XPS spectra of the C₆₀ derivative PCBM

Iulia Emilia Brumboiu, Leif Ericsson, Rickard Hansson, Ellen Moons, Olle Eriksson and Barbara Brena
J. Chem. Phys. **142**, 054306 (2015); <http://dx.doi.org/10.1063/1.4907012>

In situ formation and characterisation of singly ionised atomic europium in rare gas matrices—Luminescence spectroscopy and MP2 calculations

Owen Byrne, Barry Davis and John G. McCaffrey
J. Chem. Phys. **142**, 054307 (2015); <http://dx.doi.org/10.1063/1.4907201>

Critical evaluation of the potential energy surface of the CH₃ + HO₂ reaction system

E. P. Faragó, M. Szóri, M. C. Owen, C. Fittschen and B. Viskolcz
J. Chem. Phys. **142**, 054308 (2015); <http://dx.doi.org/10.1063/1.4907014>

Ferromagnetic spin coupling in the chromium dimer cation: Measurements by photodissociation spectroscopy combined with coupled-cluster calculations

Kazuhiro Egashira, Yurika Yamada, Yukiumi Kita and Masanori Tachikawa
J. Chem. Phys. **142**, 054309 (2015); <http://dx.doi.org/10.1063/1.4907197>

Liquids, Glasses, and Crystals

Fluid-solid coexistence from two-phase simulations: Binary colloidal mixtures and square well systems

G. Arlette Méndez-Maldonado, Gustavo A. Chapela, José Adrián Martínez-González, José Antonio Moreno, Enrique Díaz-Herrera and José Alejandro
J. Chem. Phys. **142**, 054501 (2015); <http://dx.doi.org/10.1063/1.4906424>

Liquid methanol under a static electric field

Giuseppe Cassone, Paolo V. Giaquinta, Franz Saija and A. Marco Saitta
J. Chem. Phys. **142**, 054502 (2015); <http://dx.doi.org/10.1063/1.4907010>

The wet solidus of silica: Predictions from the scaled particle theory and polarized continuum model

G. Ottonello, P. Richet and M. Vetuschi Zuccolini
J. Chem. Phys. **142**, 054503 (2015); <http://dx.doi.org/10.1063/1.4906745>

Structural and thermal investigations of an amorphous GaSe₉ alloy using EXAFS, cumulant expansion, and reverse Monte Carlo simulations

M. C. Siqueira, R. N. A. Maia, R. M. T. Araujo, K. D. Machado and S. F. Stolf
J. Chem. Phys. **142**, 054504 (2015); <http://dx.doi.org/10.1063/1.4907280>

Picosecond solvation dynamics—A potential viewer of DMSO—Water binary mixtures

Debasis Banik, Niloy Kundu, Jagannath Kuchlyan, Arpita Roy, Chiranjib Banerjee, Surajit Ghosh and Nilmoni Sarkar
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Surfaces, Interfaces, and Materials

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Determining the cohesive energy of coronene by dispersion-corrected DFT methods: Periodic boundary conditions vs. molecular pairs

J. C. Sancho-García, A. J. Pérez-Jiménez and Y. Olivier
J. Chem. Phys. **142**, 054702 (2015); <http://dx.doi.org/10.1063/1.4907268>

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Eddy Bernard, Céline Houriez, Alexander O. Mitrushchenkov, Marie Guitou and Gilberte Chambaud
J. Chem. Phys. **142**, 054703 (2015); <http://dx.doi.org/10.1063/1.4907013>

Optically probing Al—O and O—H vibrations to characterize water adsorption and surface reconstruction on α -alumina: An experimental and theoretical study

Yujin Tong, Jonas Wirth, Harald Kirsch, Martin Wolf, Peter Saalfrank and R. Kramer Campen
J. Chem. Phys. **142**, 054704 (2015); <http://dx.doi.org/10.1063/1.4906346>

Enhancing conductivity of metallic carbon nanotube networks by transition metal adsorption

T. Ketolainen, V. Havu and M. J. Puska
J. Chem. Phys. **142**, 054705 (2015); <http://dx.doi.org/10.1063/1.4907205>

Thermally driven grain boundary migration and melting in Cu

Y. H. Li, L. Wang, B. Li, J. C. E, F. P. Zhao, J. Zhu and S. N. Luo
J. Chem. Phys. **142**, 054706 (2015); <http://dx.doi.org/10.1063/1.4907272>

Study of fluorescence quenching due to 2, 3, 5, 6-tetrafluoro-7, 7', 8, 8'-tetracyano quinodimethane and its solid state diffusion analysis using photoluminescence spectroscopy

Priyanka Tyagi, Suneet Tuli and Ritu Srivastava
J. Chem. Phys. **142**, 054707 (2015); <http://dx.doi.org/10.1063/1.4907274>

Chiral selectivity of amino acid adsorption on chiral surfaces—The case of alanine on Pt

J.-H. Franke and D. S. Kosov
J. Chem. Phys. **142**, 054708 (2015); <http://dx.doi.org/10.1063/1.4907276>

Polymers and Soft Matter

Phase diagram of selectively cross-linked block copolymers shows chemically microstructured gel

Alice von der Heydt and Annette Zippelius
J. Chem. Phys. **142**, 054901 (2015); <http://dx.doi.org/10.1063/1.4905831>

Catalytic microrotor driven by geometrical asymmetry

Mingcheng Yang, Marisol Ripoll and Ke Chen
J. Chem. Phys. **142**, 054902 (2015); <http://dx.doi.org/10.1063/1.4906823>

Geometric pumping induced by shear flow in dilute liquid crystalline polymer solutions

Shunsuke Yabunaka and Hisao Hayakawa
J. Chem. Phys. **142**, 054903 (2015); <http://dx.doi.org/10.1063/1.4906557>

Phase behavior of a family of truncated hard cubes

Anjan P. Gantapara, Joost de Graaf, René van Roij and Marjolein Dijkstra
J. Chem. Phys. **142**, 054904 (2015); <http://dx.doi.org/10.1063/1.4906753>

Systematic and simulation-free coarse graining of homopolymer melts: A structure-based study

Delian Yang and Qiang Wang

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Biological Molecules and Networks

Sub-terahertz spectroscopy reveals that proteins influence the properties of water at greater distances than previously detected

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J. Chem. Phys. **142**, 055101 (2015); <http://dx.doi.org/10.1063/1.4907271>

Microscopic dynamics of water around unfolded structures of barstar at room temperature

Somedatta Pal, Kaushik Chakraborty, Prabir Khatua and Sanjoy Bandyopadhyay

J. Chem. Phys. **142**, 055102 (2015); <http://dx.doi.org/10.1063/1.4907007>

LETTERS TO THE EDITOR

Errata

Erratum: "Periodic boundary conditions for QM/MM calculations: Ewald summation for extended Gaussian basis sets" [J. Chem. Phys. 139, 244108 (2013)]

Zachary C. Holden, Ryan M. Richard and John M. Herbert

J. Chem. Phys. **142**, 059901 (2015); <http://dx.doi.org/10.1063/1.4907623>