

ARTICLES

Theoretical Methods and Algorithms

Real-space quadrature: A convenient, efficient representation for multipole expansions

David M. Rogers

J. Chem. Phys. **142**, 074101 (2015); <http://dx.doi.org/10.1063/1.4907404>

Annealed importance sampling with constant cooling rate

Edoardo Giovannelli, Gianni Cardini, Cristina Gellini, Giangaetano Pietraprerzia and Riccardo Chelli

J. Chem. Phys. **142**, 074102 (2015); <http://dx.doi.org/10.1063/1.4907883>

Improving the efficiency of branch-and-bound complete-search NMR assignment using the symmetry of molecules and spectra

Andrés Bernal, Andrés M. Castillo, Fabio González, Luc Patiny and Julien Wist

J. Chem. Phys. **142**, 074103 (2015); <http://dx.doi.org/10.1063/1.4907898>

Semiclassical quantization of nonadiabatic systems with hopping periodic orbits

Mikiya Fujii and Koichi Yamashita

J. Chem. Phys. **142**, 074104 (2015); <http://dx.doi.org/10.1063/1.4907910>

Correlation consistent basis sets for actinides. I. The Th and U atoms

Kirk A. Peterson

J. Chem. Phys. **142**, 074105 (2015); <http://dx.doi.org/10.1063/1.4907596>

Perturbations in vibrational diatomic spectra: Factorization of the molecular wave function

R. Lefebvre

J. Chem. Phys. **142**, 074106 (2015); <http://dx.doi.org/10.1063/1.4907919>

Basis convergence of range-separated density-functional theory

Odile Franck, Bastien Mussard, Eleonora Luppi and Julien Toulouse

J. Chem. Phys. **142**, 074107 (2015); <http://dx.doi.org/10.1063/1.4907920>

Chemical reactions induced by oscillating external fields in weak thermal environments

Galen T. Craven, Thomas Bartsch and Rigoberto Hernandez

J. Chem. Phys. **142**, 074108 (2015); <http://dx.doi.org/10.1063/1.4907590>

Theoretical study of a screened Hartree–Fock exchange potential using position-dependent atomic dielectric constants

Tomomi Shimazaki and Takahito Nakajima

J. Chem. Phys. **142**, 074109 (2015); <http://dx.doi.org/10.1063/1.4908061>

A localized momentum constraint for non-equilibrium molecular dynamics simulations

E. R. Smith, D. M. Heyes, D. Dini and T. A. Zaki

J. Chem. Phys. **142**, 074110 (2015); <http://dx.doi.org/10.1063/1.4907880>

Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V

Narbe Mardirossian and Martin Head-Gordon

J. Chem. Phys. **142**, 074111 (2015); <http://dx.doi.org/10.1063/1.4907719>

Local hybrid functionals with orbital-free mixing functions and balanced elimination of self-interaction error

Piotr de Silva and Clémence Corminboeuf

J. Chem. Phys. **142**, 074112 (2015); <http://dx.doi.org/10.1063/1.4908148>

Advanced Experimental Techniques

Comb-locked cavity ring-down spectrometer

Davide Gatti, Tommaso Sala, Riccardo Gotti, Lorenzo Cocola, Luca Poletto, Marco Prevedelli, Paolo Laporta and Marco Marangoni

Atoms, Molecules, and Clusters

A guided-ion beam study of the collisions and reactions of I^+ and $I+2$ with I_2

Michael L. Hause, Benjamin D. Prince and Raymond J. Bemish

J. Chem. Phys. **142**, 074301 (2015); <http://dx.doi.org/10.1063/1.4907602>

Excited state non-adiabatic dynamics of pyrrole: A time-resolved photoelectron spectroscopy and quantum dynamics study

Guorong Wu, Simon P. Neville, Oliver Schalk, Taro Sekikawa, Michael N. R. Ashfold, Graham A. Worth and Albert Stolow

J. Chem. Phys. **142**, 074302 (2015); <http://dx.doi.org/10.1063/1.4907529>

Para-hydrogen and helium cluster size distributions in free jet expansions based on Smoluchowski theory with kernel scaling

Oleg Kornilov and J. Peter Toennies

J. Chem. Phys. **142**, 074303 (2015); <http://dx.doi.org/10.1063/1.4907601>

Theoretical spectroscopic characterization at low temperatures of methyl hydroperoxide and three S-analogs

S. Dalbouha, M. L. Senent and N. Komih

J. Chem. Phys. **142**, 074304 (2015); <http://dx.doi.org/10.1063/1.4907941>

The electronic characterization of biphenylene—Experimental and theoretical insights from core and valence level spectroscopy

Johann Lüder, Monica de Simone, Roberta Totani, Marcello Coreno, Cesare Grazioli, Biplab Sanyal, Olle

Eriksson, Barbara Brena and Carla Puglia

J. Chem. Phys. **142**, 074305 (2015); <http://dx.doi.org/10.1063/1.4907723>

DFT study of Fe-Ni core-shell nanoparticles: Stability, catalytic activity, and interaction with carbon atom for single-walled carbon nanotube growth

Zhimin Yang, Qiang Wang, Xiaoye Shan, Wei-qi Li, Guang-hui Chen and Hongjun Zhu

J. Chem. Phys. **142**, 074306 (2015); <http://dx.doi.org/10.1063/1.4907897>

Mechanisms for the inversion of chirality: Global reaction route mapping of stereochemical pathways in a probable chiral extraterrestrial molecule, 2-aminopropionitrile

Ramanpreet Kaur and Vikas

J. Chem. Phys. **142**, 074307 (2015); <http://dx.doi.org/10.1063/1.4907593>

ARTICLES

Atoms, Molecules, and Clusters

Observation of the wavepacket dynamics on the $^1B_2(\Sigma_u^+)$ state of CS_2 by sub-20 fs photoelectron imaging using 159 nm probe pulses

R. Spesyvtsev, T. Horio, Y.-I. Suzuki and T. Suzuki

J. Chem. Phys. **142**, 074308 (2015); <http://dx.doi.org/10.1063/1.4907749>

Liquids, Glasses, and Crystals

Thermodynamics of fluid conduction through hydrophobic channel of carbon nanotubes: The exciting force for filling of nanotubes with polar and nonpolar fluids

Pooja Sahu, Sk. M. Ali and K. T. Shenoy

J. Chem. Phys. **142**, 074501 (2015); <http://dx.doi.org/10.1063/1.4908051>

Surfaces, Interfaces, and Materials

Improved modeling of two-dimensional transitions in dense phases on crystalline surfaces. Krypton-graphite system

E. A. Ustinov

J. Chem. Phys. **142**, 074701 (2015); <http://dx.doi.org/10.1063/1.4908035>

Liquid drops on a surface: Using density functional theory to calculate the binding potential and drop profiles and comparing with results from mesoscopic modelling

Adam P. Hughes, Uwe Thiele and Andrew J. Archer

J. Chem. Phys. **142**, 074702 (2015); <http://dx.doi.org/10.1063/1.4907732>

Structural, bonding, and electronic properties of the hexagonal ferroelectric and paraelectric phases of LuMnO₃ compound: A density functional theory study

A. M. Sousa, W. S. Coutinho, A. F. Lima and M. V. Lalic

J. Chem. Phys. **142**, 074703 (2015); <http://dx.doi.org/10.1063/1.4907787>

Influence of the van der Waals interaction in the dissociation dynamics of N₂ on W(110) from first principles

L. Martin-Gondre, J. I. Juaristi, M. Blanco-Rey, R. Díez Muiño and M. Alducin

J. Chem. Phys. **142**, 074704 (2015); <http://dx.doi.org/10.1063/1.4908060>

Facilitating guest transport in clathrate hydrates by tuning guest-host interactions

Igor L. Moudrakovski, Konstantin A. Udachin, Saman Alavi, Christopher I. Ratcliffe and John A. Ripmeester

J. Chem. Phys. **142**, 074705 (2015); <http://dx.doi.org/10.1063/1.4907720>

Coexistence and interfacial properties of a triangle-well mimicking the Lennard-Jones fluid and a comparison with noble gases

M. Bárcenas, Y. Reyes, A. Romero-Martínez, G. Odriozola and P. Orea

J. Chem. Phys. **142**, 074706 (2015); <http://dx.doi.org/10.1063/1.4909548>

Crystallinity effects on scaling properties of photoinduced modes in silver nanoprisms

Ming-Yaw Ng, I-Lin Ho and Yia-Chung Chang

J. Chem. Phys. **142**, 074707 (2015); <http://dx.doi.org/10.1063/1.4908160>

Polymers and Soft Matter

Grafted nanoparticles as soft patchy colloids: Self-assembly versus phase separation

Nathan A. Mahynski and Athanassios Z. Panagiotopoulos

J. Chem. Phys. **142**, 074901 (2015); <http://dx.doi.org/10.1063/1.4908044>

The glass transition of polymers with different side-chain stiffness confined in free-standing thin films

Shi-Jie Xie, Hu-Jun Qian and Zhong-Yuan Lu

J. Chem. Phys. **142**, 074902 (2015); <http://dx.doi.org/10.1063/1.4908047>

Simulation studies on architecture dependence of unentangled polymer melts

Xiaolei Xu, Jizhong Chen and Lijia An

J. Chem. Phys. **142**, 074903 (2015); <http://dx.doi.org/10.1063/1.4908262>

Binary mixtures of asymmetric continuous charge distributions: Molecular dynamics simulations and integral equations

D. M. Heyes and G. Rickayzen

J. Chem. Phys. **142**, 074904 (2015); <http://dx.doi.org/10.1063/1.4908046>

Cholesterics of colloidal helices: Predicting the macroscopic pitch from the particle shape and thermodynamic state

Simone Dussi, Simone Belli, René van Roij and Marjolein Dijkstra

J. Chem. Phys. **142**, 074905 (2015); <http://dx.doi.org/10.1063/1.4908162>

Biological Molecules and Networks

Vibrational energy flow in the villin headpiece subdomain: Master equation simulations

David M. Leitner, Sebastian Buchenberg, Paul Brettel and Gerhard Stock

J. Chem. Phys. **142**, 075101 (2015); <http://dx.doi.org/10.1063/1.4907881>

Dynamical role of phosphorylation on serine/threonine-proline Pin1 substrates from constant force molecular dynamics simulations

Hector A. Velazquez and Donald Hamelberg

J. Chem. Phys. **142**, 075102 (2015); <http://dx.doi.org/10.1063/1.4907884>

LETTERS TO THE EDITOR

Errata

Erratum: "Sub-terahertz spectroscopy reveals that proteins influence the properties of water at greater distances than previously detected" [J. Chem. Phys. 142, 055101 (2015)]

Oleksandr Sushko, Rostyslav Dubrovka and Robert S. Donnan

J. Chem. Phys. **142**, 079901 (2015); <http://dx.doi.org/10.1063/1.4913416>

Publisher's Note: "Geometric pumping induced by shear flow in dilute liquid crystalline polymer solutions" [J. Chem. Phys. **142, 054903 (2015)]**

Shunsuke Yabunaka and Hisao Hayakawa

J. Chem. Phys. **142**, 079902 (2015); <http://dx.doi.org/10.1063/1.4913472>