

## COMMUNICATIONS

### ***Communication: Unusual structure and transport in ionic liquid-hexane mixtures***

Min Liang, Sufia Khatun and Edward W. Castner Jr.

J. Chem. Phys. **142**, 121101 (2015); <http://dx.doi.org/10.1063/1.4916388>

### ***Communication: Improved pair approximations in local coupled-cluster methods***

Max Schwilk, Denis Usvyat and Hans-Joachim Werner

J. Chem. Phys. **142**, 121102 (2015); <http://dx.doi.org/10.1063/1.4916316>

## ARTICLES

### **Theoretical Methods and Algorithms**

#### ***Analytic second derivative of the energy for density functional theory based on the three-body fragment molecular orbital method***

Hiroya Nakata (中田浩弥), Dmitri G. Fedorov, Federico Zahariev, Michael W. Schmidt (守美都舞空), Kazuo Kitaura (北浦和夫), Mark S. Gordon (強首領真空) and Shinichiro Nakamura (中村振一郎)

J. Chem. Phys. **142**, 124101 (2015); <http://dx.doi.org/10.1063/1.4915068>

#### ***Calculation of the molecular integrals with the range-separated correlation factor***

Michał Silkowski, Michał Lesiuk and Robert Moszynski

J. Chem. Phys. **142**, 124102 (2015); <http://dx.doi.org/10.1063/1.4915272>

#### ***Time-dependent projected Hartree-Fock***

Takashi Tsuchimochi and Troy Van Voorhis

J. Chem. Phys. **142**, 124103 (2015); <http://dx.doi.org/10.1063/1.4914511>

#### ***Benchmarking DFT and semiempirical methods on structures and lattice energies for ten ice polymorphs***

Jan Gerit Brandenburg, Tilo Maas and Stefan Grimme

J. Chem. Phys. **142**, 124104 (2015); <http://dx.doi.org/10.1063/1.4916070>

#### ***Variational cross-validation of slow dynamical modes in molecular kinetics***

Robert T. McGibbon and Vijay S. Pande

J. Chem. Phys. **142**, 124105 (2015); <http://dx.doi.org/10.1063/1.4916292>

#### ***Next generation of the self-consistent and environment-dependent Hamiltonian: Applications to various boron allotropes from zero- to three-dimensional structures***

P. Tandy, Ming Yu, C. Leahy, C. S. Jayanthi and S. Y. Wu

J. Chem. Phys. **142**, 124106 (2015); <http://dx.doi.org/10.1063/1.4916069>

#### ***A transformed framework for dynamic correlation in multireference problems***

Alexander Yu. Sokolov and Garnet Kin-Lic Chan

J. Chem. Phys. **142**, 124107 (2015); <http://dx.doi.org/10.1063/1.4916315>

#### ***Soft-spring wall based non-periodic boundary conditions for non-equilibrium molecular dynamics of dense fluids***

Dhairiyashil Ghatage, Gaurav Tomar and Ratnesh K. Shukla

J. Chem. Phys. **142**, 124108 (2015); <http://dx.doi.org/10.1063/1.4916294>

#### ***Thermal transport properties of halide solid solutions: Experiments vs equilibrium molecular dynamics***

Aïmen E. Gheribi, Mathieu Salanne and Patrice Chartrand

J. Chem. Phys. **142**, 124109 (2015); <http://dx.doi.org/10.1063/1.4915524>

#### ***Natural scaling of size distributions in homogeneous and heterogeneous rate equations with size-linear capture rates***

V. G. Dubrovskii and Yu. S. Berdnikov

J. Chem. Phys. **142**, 124110 (2015); <http://dx.doi.org/10.1063/1.4916323>

#### ***Effective binary theory of multi-component nucleation***

V. I. Kalikmanov

J. Chem. Phys. **142**, 124111 (2015); <http://dx.doi.org/10.1063/1.4916356>

#### ***Surveying the free energy landscapes of continuum models: Application to soft matter systems***

Halim Kusumaatmaja

J. Chem. Phys. **142**, 124112 (2015); <http://dx.doi.org/10.1063/1.4916389>

**Functional differentiability in time-dependent quantum mechanics**

Markus Penz and Michael Ruggenthaler

J. Chem. Phys. **142**, 124113 (2015); <http://dx.doi.org/10.1063/1.4916390>

**Advanced Experimental Techniques**

**Solid-state EPR strategies for the structural characterization of paramagnetic NO adducts of frustrated Lewis pairs (FLPs)**

Marcos de Oliveira Jr., Thomas Wiegand, Lisa-Maria Elmer, Muhammad Sajid, Gerald Kehr, Gerhard Erker, Claudio José Magon and Hellmut Eckert

J. Chem. Phys. **142**, 124201 (2015); <http://dx.doi.org/10.1063/1.4916066>

**Atoms, Molecules, and Clusters**

**Applied quantum chemistry: Spectroscopic detection and characterization of the F<sub>2</sub>BS and Cl<sub>2</sub>BS free radicals in the gas phase**

Bing Jin, Phillip M. Sheridan and Dennis J. Clouthier

J. Chem. Phys. **142**, 124301 (2015); <http://dx.doi.org/10.1063/1.4915126>

**Accurate high level ab initio-based global potential energy surface and dynamics calculations for ground state of CH<sub>2</sub><sup>+</sup>**

Y. Q. Li, P. Y. Zhang and K. L. Han

J. Chem. Phys. **142**, 124302 (2015); <http://dx.doi.org/10.1063/1.4916035>

**Three-body fragmentation of CO<sub>2</sub> driven by intense laser pulses**

Chengyin Wu, Cong Wu, Yameng Fan, Xiguo Xie, Peng Wang, Yongkai Deng, Yunquan Liu and Qihuang Gong

J. Chem. Phys. **142**, 124303 (2015); <http://dx.doi.org/10.1063/1.4916045>

**The vibrational dynamics of 3D HOCl above dissociation**

Yi-Der Lin, L. E. Reichl and Christof Jung

J. Chem. Phys. **142**, 124304 (2015); <http://dx.doi.org/10.1063/1.4915142>

**Photoelectron imaging and photodissociation of ozonide in O<sub>3</sub><sup>-</sup> □ (O<sub>2</sub>)<sub>n</sub> (n = 1-4) clusters**

Jennifer E. Mann, Mary E. Troyer and Caroline Chick Jarrold

J. Chem. Phys. **142**, 124305 (2015); <http://dx.doi.org/10.1063/1.4916048>

**Differential cross sections for electron-impact vibrational-excitation of tetrahydrofuran at intermediate impact energies**

T. P. T. Do, H. V. Duque, M. C. A. Lopes, D. A. Konovalov, R. D. White, M. J. Brunger and D. B. Jones

J. Chem. Phys. **142**, 124306 (2015); <http://dx.doi.org/10.1063/1.4915888>

**The role of electron-impact vibrational excitation in electron transport through gaseous tetrahydrofuran**

H. V. Duque, T. P. T. Do, M. C. A. Lopes, D. A. Konovalov, R. D. White, M. J. Brunger and D. B. Jones

J. Chem. Phys. **142**, 124307 (2015); <http://dx.doi.org/10.1063/1.4915889>

**The hyperfine structure in the rotational spectra of D<sub>2</sub><sup>17</sup>O and HD<sup>17</sup>O: Confirmation of the absolute nuclear magnetic shielding scale for oxygen**

Cristina Puzzarini, Gabriele Cazzoli, Michael E. Harding, Juana Vázquez and Jürgen Gauss

J. Chem. Phys. **142**, 124308 (2015); <http://dx.doi.org/10.1063/1.4916068>

**Vibrational state-selective autodetachment photoelectron spectroscopy from dipole-bound states of cold 2-hydroxyphenoxide: o – HO(C<sub>6</sub>H<sub>4</sub>)O<sup>-</sup>**

Dao-Ling Huang, Hong-Tao Liu, Chuan-Gang Ning and Lai-Sheng Wang

J. Chem. Phys. **142**, 124309 (2015); <http://dx.doi.org/10.1063/1.4916122>

**Low energy elastic electron scattering from CF<sub>3</sub>Br molecules**

L. R. Hargreaves, J. R. Brunton, T. M. Maddern and M. J. Brunger

J. Chem. Phys. **142**, 124310 (2015); <http://dx.doi.org/10.1063/1.4916293>

**Adsorption of carbon monoxide on small aluminum oxide clusters: Role of the local atomic environment and charge state on the oxidation of the CO molecule**

J. C. Ornelas-Lizcano and R. A. Guirado-López

J. Chem. Phys. **142**, 124311 (2015); <http://dx.doi.org/10.1063/1.4916320>

**A novel and facile decay path of Criegee intermediates by intramolecular insertion reactions via roaming transition states**

Trong-Nghia Nguyen, Raghunath Putikam and M. C. Lin

J. Chem. Phys. **142**, 124312 (2015); <http://dx.doi.org/10.1063/1.4914987>

### ***Circular and linear magnetic birefringences in xenon at $\lambda = 1064$ nm***

Agathe Cadène, Mathilde Fouché, Alice Rivère, Rémy Battesti, Sonia Coriani, Antonio Rizzo and Carlo Rizzo  
J. Chem. Phys. **142**, 124313 (2015); <http://dx.doi.org/10.1063/1.4916049>

### ***Identification of four rotamers of m-methoxystyrene by resonant two-photon ionization and mass analyzed threshold ionization spectroscopy***

Yanqi Xu, Sheng Yuan Tzeng, Vidya Shivatare, Kaito Takahashi, Bing Zhang and Wen Bih Tzeng  
J. Chem. Phys. **142**, 124314 (2015); <http://dx.doi.org/10.1063/1.4916052>

### ***Initial mechanisms for the decomposition of electronically excited energetic materials: 1,5'-BT, 5,5'-BT, and AzTT***

Bing Yuan, Zijun Yu and Elliot R. Bernstein  
J. Chem. Phys. **142**, 124315 (2015); <http://dx.doi.org/10.1063/1.4916111>

### ***Density functional theory and chromium: Insights from the dimers***

Rolf Würdemann, Henrik H. Kristoffersen, Michael Moseler and Michael Walter  
J. Chem. Phys. **142**, 124316 (2015); <http://dx.doi.org/10.1063/1.4915265>

### ***Signatures of non-adiabatic dynamics in the fine-structure state distributions of the OH( $X^{\sim}/A^{\sim}$ ) products in the B-band photodissociation of H<sub>2</sub>O***

Linsen Zhou, Daiqian Xie and Hua Guo  
J. Chem. Phys. **142**, 124317 (2015); <http://dx.doi.org/10.1063/1.4915536>

## **Liquids, Glasses, and Crystals**

### ***Tuning structure and mobility of solvation shells surrounding tracer additives***

James Carmer, Avni Jain, Jonathan A. Bollinger, Frank van Swol and Thomas M. Truskett  
J. Chem. Phys. **142**, 124501 (2015); <http://dx.doi.org/10.1063/1.4916053>

### ***Mode coupling theory analysis of electrolyte solutions: Time dependent diffusion, intermediate scattering function, and ion solvation dynamics***

Susmita Roy, Subramanian Yashonath and Biman Bagchi  
J. Chem. Phys. **142**, 124502 (2015); <http://dx.doi.org/10.1063/1.4915274>

### ***Urea and deuterium mixtures at high pressures***

M. Donnelly, C. L. Bull, R. J. Husband, A. D. Frantzana, S. Klotz and J. S. Loveday  
J. Chem. Phys. **142**, 124503 (2015); <http://dx.doi.org/10.1063/1.4915523>

### ***Weak links between fast mobility and local structure in molecular and atomic liquids***

S. Bernini, F. Puosi and D. Leporini  
J. Chem. Phys. **142**, 124504 (2015); <http://dx.doi.org/10.1063/1.4916047>

### ***Molecular dynamics simulation of CO<sub>2</sub> hydrates: Prediction of three phase coexistence line***

J. M. Míguez, M. M. Conde, J.-P. Torrè, F. J. Blas, M. M. Piñeiro and C. Vega  
J. Chem. Phys. **142**, 124505 (2015); <http://dx.doi.org/10.1063/1.4916119>

### ***Crystallization of Lennard-Jones nanodroplets: From near melting to deeply supercooled***

Shahrazad M. A. Malek, Gregory P. Morrow and Ivan Saika-Voivod  
J. Chem. Phys. **142**, 124506 (2015); <http://dx.doi.org/10.1063/1.4915917>

### ***Decoupling of relaxation and diffusion in random pinning glass-forming liquids***

Yan-Wei Li, You-Liang Zhu and Zhao-Yan Sun  
J. Chem. Phys. **142**, 124507 (2015); <http://dx.doi.org/10.1063/1.4916208>

## **Surfaces, Interfaces, and Materials**

### ***Structures of water molecules in carbon nanotubes under electric fields***

Winarto, Daisuke Takaiwa, Eiji Yamamoto and Kenji Yasuoka  
J. Chem. Phys. **142**, 124701 (2015); <http://dx.doi.org/10.1063/1.4914462>

### ***Characterization of adsorbed water in MIL-53(Al) by FTIR spectroscopy and ab-initio calculations***

J. M. Salazar, G. Weber, J. M. Simon, I. Bezverkhyy and J. P. Bellat  
J. Chem. Phys. **142**, 124702 (2015); <http://dx.doi.org/10.1063/1.4914903>

### ***Opening gates to oxygen reduction reactions on Cu(111) surface***

Aslihan Sumer and Santanu Chaudhuri  
J. Chem. Phys. **142**, 124703 (2015); <http://dx.doi.org/10.1063/1.4914901>

### ***A first-principles study of Pt thin films on SrTiO<sub>3</sub>(100): Support effects on CO adsorption***

Simuck F. Yuk and Aravind Asthagiri  
J. Chem. Phys. **142**, 124704 (2015); <http://dx.doi.org/10.1063/1.4915521>

### ***Electrolyte pore/solution partitioning by expanded grand canonical ensemble Monte Carlo simulation***

Filip Moucka, Dusan Bratko and Alenka Luzar

J. Chem. Phys. **142**, 124705 (2015); <http://dx.doi.org/10.1063/1.4914461>

**Structure and dynamics of POPC bilayers in water solutions of room temperature ionic liquids**

Antonio Benedetto, Richard J. Bingham and Pietro Ballone

J. Chem. Phys. **142**, 124706 (2015); <http://dx.doi.org/10.1063/1.4915918>

**Polymers and Soft Matter**

**Effects of the internal friction and the solvent quality on the dynamics of a polymer chain closure**

Wancheng Yu and Kaifu Luo

J. Chem. Phys. **142**, 124901 (2015); <http://dx.doi.org/10.1063/1.4915927>

**Small membranes under negative surface tension**

Yotam Y. Avital and Oded Farago

J. Chem. Phys. **142**, 124902 (2015); <http://dx.doi.org/10.1063/1.4915512>

**Regulating block copolymer phases via selective homopolymers**

Shuang Yang, Zhen Lei, Nan Hu, Er-Qiang Chen and An-Chang Shi

J. Chem. Phys. **142**, 124903 (2015); <http://dx.doi.org/10.1063/1.4915538>

**Excluded volume effects in compressed polymer brushes: A density functional theory**

Cangyi Chen, Ping Tang, Feng Qiu and An-Chang Shi

J. Chem. Phys. **142**, 124904 (2015); <http://dx.doi.org/10.1063/1.4916133>

**How does a flexible chain of active particles swell?**

Andreas Kaiser, Sonja Babel, Borge ten Hagen, Christian von Ferber and Hartmut Löwen

J. Chem. Phys. **142**, 124905 (2015); <http://dx.doi.org/10.1063/1.4916134>

**Biological Molecules and Networks**

**DNA-binding protein searches for its target: Non-monotonic dependence of the search time on the density of roadblocks bound on the DNA chain**

Lin Liu and Kaifu Luo

J. Chem. Phys. **142**, 125101 (2015); <http://dx.doi.org/10.1063/1.4916056>

**Dependence of FRET efficiency on distance in single donor-acceptor pairs**

I. S. Osad'ko

J. Chem. Phys. **142**, 125102 (2015); <http://dx.doi.org/10.1063/1.4915279>

**Flexibility of short DNA helices with finite-length effect: From base pairs to tens of base pairs**

Yuan-Yan Wu, Lei Bao, Xi Zhang and Zhi-Jie Tan

J. Chem. Phys. **142**, 125103 (2015); <http://dx.doi.org/10.1063/1.4915539>

**Isotope-enriched protein standards for computational amide I spectroscopy**

Mike Reppert, Anish R. Roy and Andrei Tokmakoff

J. Chem. Phys. **142**, 125104 (2015); <http://dx.doi.org/10.1063/1.4915271>

**Increasing the sampling efficiency of protein conformational transition using velocity-scaling optimized hybrid explicit/implicit solvent REMD simulation**

Yuqi Yu, Jinan Wang, Qiang Shao, Jiye Shi and Weiliang Zhu

J. Chem. Phys. **142**, 125105 (2015); <http://dx.doi.org/10.1063/1.4916118>

**LETTERS TO THE EDITOR**

**Errata**

**Publisher's Note: "Unusual behavior in magnesium-copper cluster matter produced by helium droplet mediated deposition" [J. Chem. Phys. **142**, 084307 (2015)]**

S. B. Emery, Y. Xin, C. J. Ridge, R. J. Buszek, J. A. Boatz, J. M. Boyle, B. K. Little and C. M. Lindsay

J. Chem. Phys. **142**, 129901 (2015); <http://dx.doi.org/10.1063/1.4916117>

**Publisher's Note: "The total position-spread tensor: Spin partition" [J. Chem. Phys. **142**, 094113 (2015)]**

Muammar El Khatib, Oriana Brea, Edoardo Fertitta, Gian Luigi Bendazzoli, Stefano Evangelisti and Thierry Leininger

J. Chem. Phys. **142**, 129902 (2015); <http://dx.doi.org/10.1063/1.4916357>

**Erratum: "Electron impact excitation of the low-lying  $3s[3/2]_1$  and  $3s'[1/2]_1$  levels in neon for incident energies between 20 and 300 eV" [J. Chem. Phys. **139**, 184301 (2013)]**

M. Hoshino, H. Murai, H. Kato, M. J. Brunger, Y. Itikawa and H. Tanaka

J. Chem. Phys. **142**, 129903 (2015); <http://dx.doi.org/10.1063/1.4916381>

**Erratum: "The  $PtAl$  and  $PtAl_2^-$  anions: Theoretical and photoelectron spectroscopic characterization" [J. Chem. Phys. **140**, 164316 (2014)]**

Xinxing Zhang, Gerd Ganteför, Kit H. Bowen and Anastassia N. Alexandrova

J. Chem. Phys. **142**, 129904 (2015); <http://dx.doi.org/10.1063/1.4916639>

## LETTERS TO THE EDITOR

### Errata

**Erratum: “Electronic couplings for molecular charge transfer: Benchmarking CDFT, FODFT, and FODFTB against high-level *ab initio* calculations” [J. Chem. Phys. **140**, 104105 (2014)]**

Adam Kubas, Felix Hoffmann, Alexander Heck, Harald Oberhofer, Marcus Elstner and Jochen Blumberger

J. Chem. Phys. **142**, 129905 (2015); <http://dx.doi.org/10.1063/1.4916382>