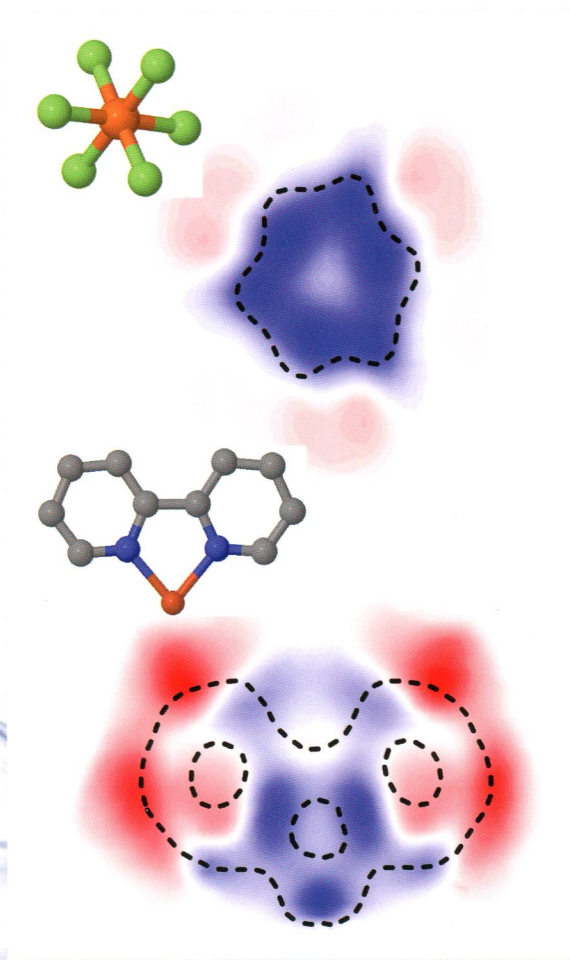


14 January 2014

Volume 140 Number 2

TM
J80/cp

AIP | The Journal of Chemical Physics



jcp.aip.org

► Cover image from T. Elsaesser and M. Woerner, *J. Chem. Phys.* **140**, 020901 (2014).

PERSPECTIVES

Perspective: Structural dynamics in condensed matter mapped by femtosecond x-ray diffraction (11 pages)
T. Elsaesser and M. Woerner 020901

ARTICLES

Theoretical Methods and Algorithms

- Excitation energies with linear response density matrix functional theory along the dissociation coordinate of an electron-pair bond in N -electron systems (19 pages)**
R. van Meer, O. V. Gritsenko, and E. J. Baerends 024101
- Analysis of and remedies for unphysical ground states of the multireference averaged coupled-pair functional (5 pages)**
David B. Krisiloff, Victor B. Oyeyemi, Florian Libisch, and Emily A. Carter 024102
- Nuclear quadrupole moment-induced Cotton-Mouton effect in molecules (13 pages)**
Li-juan Fu and Juha Vaara 024103
- A method for analyzing the non-stationary nucleation and overall transition kinetics: A case of water (6 pages)**
Anatolii V. Mokshin and Bulat N. Galimzyanov 024104
- Multilevel summation for dispersion: A linear-time algorithm for r^{-6} potentials (12 pages)**
Daniel Tameling, Paul Springer, Paolo Bientinesi, and Ahmed E. Ismail 024105
- Numerical approach to unbiased and driven generalized elastic model (9 pages)**
M. Ghasemi Nezhadhighi, A. Checkkin, and R. Metzler 024106
- Imaginary time correlations and the phaseless auxiliary field quantum Monte Carlo (12 pages)**
M. Motta, D. E. Galli, S. Moroni, and E. Vitali 024107
- Linear response theory for the density matrix renormalization group: Efficient algorithms for strongly correlated excited states (13 pages)**
Naoki Nakatani, Sebastian Wouters, Dimitri Van Neck, and Garnet Kin-Lic Chan 024108
- Dissecting molecular descriptors into atomic contributions in density functional reactivity theory (9 pages)**
Chunying Rong, Tian Lu, and Shubin Liu 024109
- Electron transfer in a two-level system within a Cole-Davidson vitreous bath (6 pages)**
Mehdi Zarea, Mark A. Ratner, and Michael R. Wasielewski 024110
- Stochastic, real-space, imaginary-time evaluation of third-order Feynman–Goldstone diagrams (7 pages)**
Soohaeng Yoo Willow and So Hirata 024111
- Fitting coupled potential energy surfaces for large systems: Method and construction of a 3-state representation for phenol photodissociation in the full 33 internal degrees of freedom using multireference configuration interaction determined data (21 pages)**
Xiaolei Zhu and David R. Yarkony 024112

(Continued)

A1

Федеральное государственное
бюджетное учреждение науки
Центральная научная библиотека
Уральского отделения
Российской академии наук (ЦНБ УрО РАН)

© 2014 AIP Publishing LLC

Atoms, Molecules, and Clusters

Prediction of 1P Rydberg energy levels of beryllium based on calculations with explicitly correlated Gaussians (5 pages)	024301
Sergiy Bubin and Ludwik Adamowicz	
Photo-fragmentation spectroscopy of benzylum and 1-phenylethyl cations (10 pages)	024302
Géraldine Féraud, Claude Dedonder-Lardeux, Satchin Soorkia, and Christophe Jouvet	
Electronic structure and reactivity in water splitting of the iron oxide dimers and their hexacarbonyls: A density functional study (12 pages)	024303
Ellie L. Uzunova and Hans Mikosch	
A relativistic time-dependent density functional study of the excited states of the mercury dimer (14 pages)	024304
Ossama Kullie	
Parity violation in nuclear magnetic resonance frequencies of chiral tetrahedral tungsten complexes NWXYZ (X, Y, Z = H, F, Cl, Br or I) (7 pages)	024305
Sophie Nahrwold, Robert Berger, and Peter Schwerdtfeger	
Investigating the significance of zero-point motion in small molecular clusters of sulphuric acid and water (6 pages)	024306
Jake L. Stinson, Shawn M. Kathmann, and Ian J. Ford	
The permanent electric dipole moment of thorium sulfide, ThS (5 pages)	024307
Anh Le, Michael C. Heaven, and Timothy C. Steimle	
Smallest fullerene-like silicon cage stabilized by a V_2 unit (5 pages)	024308
Hong-Guang Xu, Xiang-Yu Kong, Xiao-Jiao Deng, Zeng-Guang Zhang, and Wei-Jun Zheng	
An improved model electronic Hamiltonian for potential energy surfaces and spin-orbit couplings of low-lying d-d states of $[\text{Fe}(\text{bpy})_3]^{2+}$ (11 pages)	024309
Satoru Iuchi and Nobuaki Koga	
Product fine-structure resolved photodissociation dynamics: The A band of H_2O (9 pages)	024310
Linsen Zhou, Daiqian Xie, Zhigang Sun, and Hua Guo	
The effect of classical and quantum dynamics on vibrational frequency shifts of H_2 in clathrate hydrates (11 pages)	024311
Nuria Plattner and Markus Meuwly	
Reduced dimension rovibrational variational calculations of the S_1 state of C_2H_2. I. Methodology and implementation (12 pages)	024312
P. Bryan Changala	
Reduced dimension rovibrational variational calculations of the S_1 state of C_2H_2. II. The S_1 rovibrational manifold and the effects of isomerization (9 pages)	024313
P. Bryan Changala, Joshua H. Baraban, John F. Stanton, Anthony J. Merer, and Robert W. Field	
Positive and negative ion formation in deep-core excited molecules: S 1s excitation in dimethyl sulfoxide (8 pages)	024314
L. H. Coutinho, D. J. Gardenghi, A. S. Schlachter, G. G. B. de Souza, and W. C. Stolte	
Protonation effect on the electronic properties of 2-pyridone monomer, dimer and its water clusters: A theoretical study (10 pages)	024315
Behnaz Saed and Reza Omidyan	
Time- and frequency-dependent model of time-resolved coherent anti-Stokes Raman scattering (CARS) with a picosecond-duration probe pulse (16 pages)	024316
Hans U. Stauffer, Joseph D. Miller, Mikhail N. Slipchenko, Terrence R. Meyer, Benjamin D. Prince, Suresh Roy, and James R. Gord	

(Continued)

Shape resonance spectra of uracil, 5-fluorouracil, and 5-chlorouracil (7 pages) F. Kossoski, M. H. F. Bettega, and M. T. do N. Varella	024317
Wave function for harmonically confined electrons in time-dependent electric and magnetostatic fields (9 pages) Hong-Ming Zhu, Jin-Wang Chen, Xiao-Yin Pan, and Virahat Sahni	024318
The influence of a presence of a heavy atom on the spin-spin coupling constants between two light nuclei in organometallic compounds and halogen derivatives (8 pages) Artur Wodyński and Magdalena Pecul	024319

Liquids, Glasses, and Crystals

Turing-Hopf instabilities through a combination of diffusion, advection, and finite size effects (6 pages) Sainyam Galhotra, J. K. Bhattacharjee, and Bijay Kumar Agarwalla	024501
The application of the integral equation theory to study the hydrophobic interaction (6 pages) Tomaž Mohorič, Tomaz Urbic, and Barbara Hribar-Lee	024502
Anisotropy of singlet exciton diffusion in organic semiconductor crystals from <i>ab initio</i> approaches (12 pages) V. Stehr, B. Engels, C. Deibel, and R. F. Fink	024503
Reverse Monte Carlo modeling in confined systems (9 pages) V. Sánchez-Gil, E. G. Noya, and E. Lomba	024504
A transition state theory for calculating hopping times and diffusion in highly confined fluids (7 pages) Surajith N. Wanasundara, Raymond J. Spiteri, and Richard K. Bowles	024505
Continuous distributions of charges: Extensions of the one component plasma (10 pages) D. M. Heyes and G. Rickayzen	024506

Surfaces, Interfaces, and Materials

Electronic structure changes during the surface-assisted formation of a graphene nanoribbon (7 pages) Christopher Bronner, Manuel Utecht, Anton Haase, Peter Saalfrank, Tillmann Klamroth, and Petra Tegeder	024701
Finite-temperature second-order many-body perturbation and Hartree–Fock theories for one-dimensional solids: An application to Peierls and charge-density-wave transitions in conjugated polymers (7 pages) Xiao He, Shinsei Ryu, and So Hirata	024702
Calculation of the interfacial free energy of a binary hard-sphere fluid at a planar hard wall (7 pages) Jesse L. Kern and Brian B. Laird	024703
Thermodynamic stability of nanosized multicomponent bubbles/droplets: The square gradient theory and the capillary approach (9 pages) Øivind Wilhelmsen, Dick Bedeaux, Signe Kjelstrup, and David Reguera	024704
Solid phases of spatially nanoconfined oxygen: A neutron scattering study (9 pages) Danny Kojda, Dirk Wallacher, Simon Baudoin, Thomas Hansen, Patrick Huber, and Tommy Hofmann	024705
Temperature effects on adsorption and diffusion dynamics of $\text{CH}_3\text{CH}_{2(\text{ads})}$ and $\text{H}_3\text{C}-\text{C}\equiv\text{C}_{(\text{ads})}$ on Ag(111) surface and their self-coupling reactions: <i>Ab initio</i> molecular dynamics approach (11 pages) Shao-Yu Lu and Jyh-Shing Lin	024706
Nitrogen-induced reconstruction and faceting of Re(11$\bar{2}$1) (7 pages) Hao Wang, Wenhua Chen, Robert A. Bartynski, Payam Kaghazchi, and Timo Jacob	024707

A kinetic model for heterogeneous condensation of vapor on an insoluble spherical particle (8 pages) Xisheng Luo, Yu Fan, Fenghua Qin, Huaqiao Gui, and Jianguo Liu	024708
Second order classical perturbation theory for atom surface scattering: Analysis of asymmetry in the angular distribution (10 pages) Yun Zhou (周匀), Eli Pollak, and Salvador Miret-Artés	024709
Polymers and Soft Matter	
Generalized Onsager theory for strongly anisometric patchy colloids (13 pages) H. H. Wensink and E. Trizac	024901
Molecular dynamics simulations of shock waves in hydroxyl-terminated polybutadiene melts: Mechanical and structural responses (12 pages) Markus G. Fröhlich, Thomas D. Sewell, and Donald L. Thompson	024902
Shape variation of micelles in polymer thin films (9 pages) Jiajia Zhou and An-Chang Shi	024903
Organization of polymer chains onto long, single-wall carbon nano-tubes: Effect of tube diameter and cooling method (14 pages) Sunil Kumar, Sudip K. Pattanayek, and Gerald G. Pereira	024904
Coherent states formulation of polymer field theory (13 pages) Xingkun Man, Kris T. Delaney, Michael C. Villet, Henri Orland, and Glenn H. Fredrickson	024905
Effects of ionic liquids on cation dynamics in amorphous polyethylene oxide electrolytes (6 pages) Joyjit Chattoraj, Diddo Diddens, and Andreas Heuer	024906
Rigidity of a spherical capsule switches the localization of encapsulated particles between inner and peripheral regions under crowding condition: Simple model on cellular architecture (9 pages) Chwen-Yang Shew, Kenta Kondo, and Kenichi Yoshikawa	024907
Revisit to phase diagram of poly(<i>N</i>-isopropylacrylamide) microgel suspensions by mechanical spectroscopy (6 pages) Huaguang Wang, Xuebang Wu, Zhengang Zhu, C. S. Liu, and Zexin Zhang	024908
Slow dynamics of nanocomposite polymer aerogels as revealed by X-ray photocalorrelation spectroscopy (XPCS) (6 pages) Rebeca Hernández, Aurora Nogales, Michael Sprung, Carmen Mijangos, and Tiberio A. Ezquerro	024909
Born energy, acid-base equilibrium, structure and interactions of end-grafted weak polyelectrolyte layers (15 pages) R. J. Nap, M. Tagliacucchi, and I. Szleifer	024910
Study of the B1-B2 transition in colloidal clusters (7 pages) D. Bochicchio, A. Videcoq, and R. Ferrando	024911
Entropic force on granular chains self-extracting from one-dimensional confinement (5 pages) Pei-Ren Jeng, KuanHua Chen, Gwo-jen Hwang, Ethan Y. Cho, Chenhsin Lien, Kiwing To, and Y. C. Chou	024912
Biological Molecules and Networks	
Kinks, loops, and protein folding, with protein A as an example (17 pages) Andrey Krokhotin, Adam Liwo, Gia G. Maisuradze, Antti J. Niemi, and Harold A. Scheraga	025101
Kinetic partitioning mechanism of HDV ribozyme folding (12 pages) Jiawen Chen, Sha Gong, Yujie Wang, and Wenbing Zhang	025102

(Continued)

A cascade through spin states in the ultrafast haem relaxation of met-myoglobin (8 pages)
Cristina Consani, Gerald Auböck, Olivier Bräm, Frank van Mourik, and Majed Chergui 025103

LETTERS TO THE EDITOR

Notes

Note: Depletion potentials in non-additive asymmetric binary mixtures of hard-spheres (2 pages)
César D. Estrada-Alvarez, Erik López-Sánchez, Gabriel Pérez-Ángel, Pedro González-Mozuelos,
José Miguel Méndez-Alcaraz, and Ramón Castañeda-Priego 026101