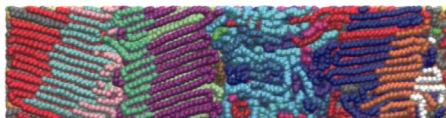
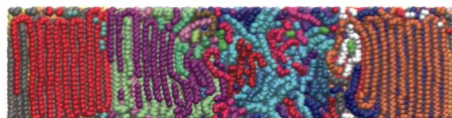
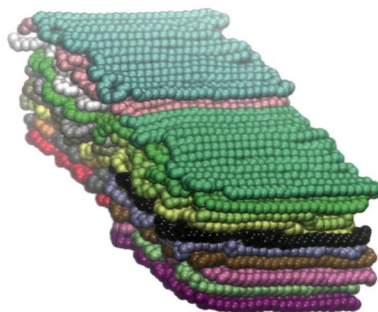
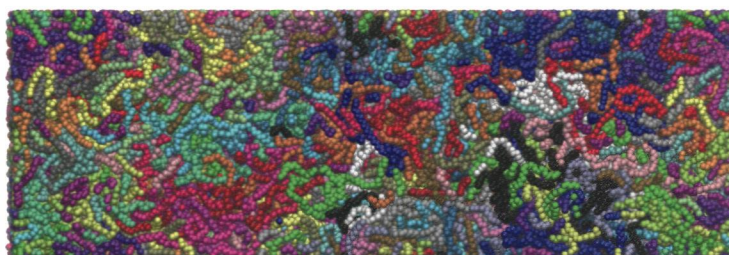


21 April 2014

Volume 140 Number 15

NU
J80/cp

AIP | The Journal of Chemical Physics



► Cover image from Y. Wang, D. MacKernan, D. Cubero, D. F. Coker, and N. Quirke, *J. Chem. Phys.* **140**, 154902 (2014).

COMMUNICATIONS

- Communication: A benchmark-quality, full-dimensional *ab initio* potential energy surface for Ar-HOCO (5 pages)**
Riccardo Conte, Paul L. Houston, and Joel M. Bowman 151101
- Communication: Disorder-suppressed vibrational relaxation in vapor-deposited high-density amorphous ice (5 pages)**
Andrey Shalit, Fivos Perakis, and Peter Hamm 151102

ARTICLES

Theoretical Methods and Algorithms

- The rigorous stochastic matrix multiplication scheme for the calculations of reduced equilibrium density matrices of open multilevel quantum systems (12 pages)**
Xin Chen 154101
- Optimized coordinates in vibrational coupled cluster calculations (15 pages)**
Bo Thomsen, Kiyoshi Yagi, and Ove Christiansen 154102
- Can the ring polymer molecular dynamics method be interpreted as real time quantum dynamics? (11 pages)**
Seogjoo Jang, Anton V. Sinitskiy, and Gregory A. Voth 154103
- Determination of the Eckart molecule-fixed frame by use of the apparatus of quaternion algebra (7 pages)**
Sergey V. Krasnoshchekov, Elena V. Isayeva, and Nikolay F. Stepanov 154104
- Modeling the adsorption of short alkanes in the zeolite SSZ-13 using “van der Waals” DFT exchange correlation functionals: Understanding the advantages and limitations of such functionals (4 pages)**
Florian Göttl and Philippe Sautet 154105
- On equivalence of high temperature series expansion and coupling parameter series expansion in thermodynamic perturbation theory of fluids (5 pages)**
A. Sai Venkata Ramana 154106
- Exploration of zeroth-order wavefunctions and energies as a first step toward intramolecular symmetry-adapted perturbation theory (10 pages)**
Jérôme F. Gonthier and Clémence Corminboeuf 154107
- Finite barrier corrections to the PGH solution of Kramers’ turnover theory (16 pages)**
Eli Pollak and Reuven Ianconescu 154108
- Distance fluctuation of a single molecule in Lennard-Jones liquid based on generalized Langevin equation and mode coupling theory (9 pages)**
Ping Li, Yunhong Dong, Nanrong Zhao, and Zhonghuai Hou 154109

Atoms, Molecules, and Clusters

- State-resolved imaging of CO from propenal photodissociation: Signatures of concerted three-body dissociation (7 pages)**
Arghya Dey, Ravin Fernando, and Arthur G. Suits 154301

Far-infrared collision-induced absorption in rare gas mixtures: Quantum and semi-classical calculations (8 pages)	
Ilya Buryak, Lothar Frommhold, and Andrey A. Vigasin	154302
Accurate non-Born-Oppenheimer calculations of the complete pure vibrational spectrum of ditritium using all-particle explicitly correlated Gaussian functions (5 pages)	
Sergiy Bubin, Monika Stanke, and Ludwik Adamowicz	154303
A diabatic representation of the two lowest electronic states of Li₃ (10 pages)	
Elham Nour Ghassemi, Jonas Larson, and Åsa Larson	154304
Effect of antisymmetric C–H stretching excitation on the dynamics of O(¹D) + CH₄ → OH + CH₃ (9 pages)	
Huilin Pan, Jiayue Yang, Dong Zhang, Quan Shuai, Dongxu Dai, Guorong Wu, Bo Jiang, and Xueming Yang	154305
Thermal decomposition of 1,3,3-trinitroazetidine (TNAZ): A density functional theory and <i>ab initio</i> study (10 pages)	
Jeffrey D. Veals and Donald L. Thompson	154306
Rationalizing the role of structural motif and underlying electronic structure in the finite temperature behavior of atomic clusters (7 pages)	
Anju Susan and Kavita Joshi	154307
Density functional calculations for structural, electronic, and magnetic properties of gadolinium-oxide clusters (14 pages)	
H. K. Yuan, H. Chen, C. L. Tian, A. L. Kuang, and J. Z. Wang	154308
Mesoscale properties of clay aggregates from potential of mean force representation of interactions between nanoplatelets (17 pages)	
Davoud Ebrahimi, Andrew J. Whittle, and Roland J.-M. Pellenq	154309
The intensity of forbidden torsional transitions in electronic spectra of molecules with a 6-fold barrier: Application to toluenes (13 pages)	
Edwina A. Virgo, Jason R. Gascooke, and Warren D. Lawrance	154310
Liquids, Glasses, and Crystals	
A model for phosphate glass topology considering the modifying ion sub-network (8 pages)	
Christian Hermansen, John C. Mauro, and Yuanzheng Yue	154501
The role of the anisotropy on the solid-fluid phase transition in core-softened shoulder-dumbbells systems (8 pages)	
Cristina Gavazzoni, Guilherme K. Gonzatti, Luiz Felipe Pereira, Luis Henrique Coelho Ramos, Paulo A. Netz, and Marcia C. Barbosa	154502
Anisotropic orbital occupation and Jahn-Teller distortion of orthorhombic YMnO₃ epitaxial films: A combined experimental and theoretical study on polarization-dependent x-ray absorption spectroscopy (4 pages)	
Shu-Chih Haw, Jenn-Min Lee, Shin-Ann Chen, Kueih-Tzu Lu, Pao-An Lin, Chih-Hao Lee, Ming-Tao Lee, Tun-Wen Pi, Zhiwei Hu, and Jin-Ming Chen	154503
Structural and elastic properties of a hypothetical high density <i>sp</i>²-rich amorphous carbon phase (7 pages)	
L. L. Wang and M. Zhao	154504
Anomalous properties of water predicted by the BK3 model (5 pages)	
Péter T. Kiss and András Baranyai	154505
A diagrammatic kinetic theory of density fluctuations in simple liquids in the overdamped limit. I. A long time scale theory for high density (25 pages)	
Kevin R. Pilkiewicz and Hans C. Andersen	154506

A diagrammatic kinetic theory of density fluctuations in simple liquids in the overdamped limit.

II. The one-loop approximation (13 pages)

Kevin R. Pilkiewicz and Hans C. Andersen 154507

Influence of electric fields on the structure and structure transition of water confined in a carbon nanotube (7 pages)

Zhenyu Qian, Zhaoming Fu, and Guanghong Wei 154508

Surfaces, Interfaces, and Materials

Analytical model for the effects of wetting on thermal boundary conductance across solid/classical liquid interfaces (7 pages)

Matthew E. Caplan, Ashutosh Giri, and Patrick E. Hopkins 154701

Real-time x-ray scattering study of the initial growth of organic crystals on polymer brushes (7 pages)

Sung Yup An, Kwangseok Ahn, Doris Yangsoo Kim, Hyun-Hwi Lee, Jeong Ho Cho, and Dong Ryeol Lee 154702

Electric double layer for a size-asymmetric electrolyte around a spherical colloid (9 pages)

Eun-Young Kim and Soon-Chul Kim 154703

Polymers and Soft Matter

Self-consistent electric field-induced dipole interaction of colloidal spheres, cubes, rods, and dumbbells (12 pages)

Bas W. Kwaadgras, René van Roij, and Marjolein Dijkstra 154901

Single electron states in polyethylene (11 pages)

Y. Wang, D. MacKernan, D. Cubero, D. F. Coker, and N. Quirke 154902

Accurate phase diagram of tetravalent DNA nanostars (10 pages)

Lorenzo Rovigatti, Francesca Bomboi, and Francesco Sciortino 154903

Depletion interaction between two ellipsoids (6 pages)

Han Miao, Yao Li, and Hongru Ma 154904

Biological Molecules and Networks

DNA strand breaks and crosslinks induced by transient anions in the range 2-20 eV (11 pages)

Xinglan Luo, Yi Zheng, and Léon Sanche 155101

NMR spin relaxation in proteins: The patterns of motion that dissipate power to the bath (16 pages)

Yury E. Shapiro and Eva Meirovitch 155102

Simulation study of the effects of surface chemistry and temperature on the conformations of ssDNA oligomers near hydrophilic and hydrophobic surfaces (14 pages)

Robert M. Elder and Arthi Jayaraman 155103

LETTERS TO THE EDITOR

Notes

Note: On the evaporation coefficient of water (2 pages)

Michael A. Bellucci and Bernhardt L. Trout 156101