

AIP | **The Journal of
Chemical Physics**



► **Cover image** from A. A. Glagoleva, V. V. Vasilevskaya, K. Yoshikawa, and A. R. Khokhlov, *J. Chem. Phys.* **139**, 244901 (2013).

COMMUNICATIONS

Communication: Non-monotonic supersaturation dependence of the nucleus size of crystals with anisotropically interacting molecules (4 pages)

R. J. Bingham, L. G. Rizzi, R. Cabriolu, and S. Auer 241101

ARTICLES

Theoretical Methods and Algorithms

Phonon interference effects in molecular junctions (10 pages)

Troels Markussen 244101

Multicomponent dynamics of coupled quantum subspaces and field-induced molecular ionizations (16 pages)

Thanh-Tung Nguyen-Dang and Jérémy Viau-Trudel 244102

Fixman compensating potential for general branched molecules (11 pages)

Abhinandan Jain, Saugat Kandel, Jeffrey Wagner, Adrien Larsen, and Nagarajan Vaidehi 244103

Propensity approach to nonequilibrium thermodynamics of a chemical reaction network: Controlling single E-coli β -galactosidase enzyme catalysis through the elementary reaction steps (8 pages)

Biswajit Das, Kinshuk Banerjee, and Gautam Gangopadhyay 244104

Higher-order electric multipole contributions to retarded non-additive three-body dispersion interaction energies between atoms: Equilateral triangle and collinear configurations (11 pages)

A. Salam 244105

Multiple time step molecular dynamics in the optimized isokinetic ensemble steered with the molecular theory of solvation: Accelerating with advanced extrapolation of effective solvation forces (23 pages)

Igor Omelyan and Andriy Kovalenko 244106

Analytical energy gradient based on spin-free infinite-order Douglas-Kroll-Hess method with local unitary transformation (13 pages)

Yuya Nakajima, Junji Seino, and Hiromi Nakai 244107

Periodic boundary conditions for QM/MM calculations: Ewald summation for extended Gaussian basis sets (13 pages)

Zachary C. Holden, Ryan M. Richard, and John M. Herbert 244108

Regularized orbital-optimized second-order perturbation theory (7 pages)

David Stück and Martin Head-Gordon 244109

Two-photon spectroscopy of excitons with entangled photons (11 pages)

Frank Schlawin and Shaul Mukamel 244110

Frequency-domain multiscale quantum mechanics/electromagnetics simulation method (6 pages)

Lingyi Meng, Zhenyu Yin, ChiYung Yam, SiuKong Koo, Quan Chen, Ngai Wong, and GuanHua Chen 244111

Advanced Experimental Techniques

- Coherent transfer of nuclear spin polarization in field-cycling NMR experiments (12 pages)**
 Andrey N. Pravdivtsev, Alexandra V. Yurkovskaya, Hans-Martin Vieth, and Konstantin L. Ivanov 244201
- Formation of ionic complexes in cryogenic matrices: A case study using co-deposition of Cu⁻ with rare gas cations in solid argon (9 pages)**
 Ryan M. Ludwig and David T. Moore 244202

Atoms, Molecules, and Clusters

- Fourier-transform spectroscopy of $(4)^1\Sigma^+ \rightarrow A^1\Sigma^+ - b^3\Pi$, $A^1\Sigma^+ - b^3\Pi \rightarrow X^1\Sigma^+$, and $(1)^3\Delta_1 \rightarrow b^3\Pi_{0\pm}$ transitions in KCs and deperturbation treatment of $A^1\Sigma^+$ and $b^3\Pi$ states (14 pages)**
 A. Kruzins, I. Klincare, O. Nikolayeva, M. Tamanis, R. Ferber, E. A. Pazyuk, and A. V. Stolyarov 244301
- A revisit of the Förster energy transfer near a metallic spherical nanoparticle: (1) Efficiency enhancement or reduction? (2) The control of the Förster radius of the unbounded medium. (3) The impact of the local density of states (15 pages)**
 J. Alejandro Gonzaga-Galeana and Jorge R. Zurita-Sánchez 244302
- Probing the electronic structures of low oxidation-state uranium fluoride molecules UF_x^- ($x = 2-4$) (8 pages)**
 Wei-Li Li, Han-Shi Hu, Tian Jian, Gary V. Lopez, Jing Su, Jun Li, and Lai-Sheng Wang 244303
- A non-adiabatic dynamics study of octatetraene: The radiationless conversion from S_2 to S_1 (9 pages)**
 Zexing Qu and Chungeng Liu 244304
- Synchrotron-based far infrared study of the rotation-vibration-inversion spectrum of silacyclobutane below 500 cm^{-1} : The ν_{29} and ν_{30} bands (10 pages)**
 Ziqiu Chen and Jennifer van Wijngaarden 244305
- Density functional theory study of the interaction of vinyl radical, ethyne, and ethene with benzene, aimed to define an affordable computational level to investigate stability trends in large van der Waals complexes (16 pages)**
 Andrea Maranzana, Anna Giordana, Antonius Indarto, Glauco Tonachini, Vincenzo Barone, Mauro Causà, and Michele Pavone 244306
- Electron tunneling characteristics of a cubic quantum dot, $(PbS)_{32}$ (5 pages)**
 Sanjeev K. Gupta, Haiying He, Douglas Banyai, Anil K. Kandalam, and Ravindra Pandey 244307
- ^{33}S hyperfine interactions in H_2S and SO_2 and revision of the sulfur nuclear magnetic shielding scale (9 pages)**
 Trygve Helgaker, Jürgen Gauss, Gabriele Cazzoli, and Cristina Puzzarini 244308
- A full dimensional investigation of infrared spectroscopy of the RbCs dimer using the multi-configuration time-dependent Hartree method (8 pages)**
 Huihui Wang, Yonggang Yang, Liantuan Xiao, and Suotang Jia 244309
- Spectroscopic observation of higher vibrational levels of C_2 through visible band systems (9 pages)**
 Masakazu Nakajima and Yasuki Endo 244310
- Multi-photon ionization and fragmentation of uracil: Neutral excited-state ring opening and hydration effects (10 pages)**
 B. Barc, M. Ryszka, J. Spurrell, M. Dampc, P. Limão-Vieira, R. Parajuli, N. J. Mason, and S. Eden 244311
- Structure, stability, and electronic property of carbon-doped gold clusters Au_nC^- ($n = 1-10$): A density functional theory study (12 pages)**
 Li-Li Yan, Yi-Rong Liu, Teng Huang, Shuai Jiang, Hui Wen, Yan-Bo Gai, Wei-Jun Zhang, and Wei Huang 244312

(Continued)

Liquids, Glasses, and Crystals

- Effect of chain flexibility on master curve behavior for diffusion coefficient (6 pages)**
 Joanne Budzien, Julieanne V. Heffernan, and John D. McCoy 244501
- ESR lineshape and ^1H spin-lattice relaxation dispersion in propylene glycol solutions of nitroxide radicals – Joint analysis (12 pages)**
 D. Kruk, S. K. Hoffmann, J. Goslar, S. Lijewski, A. Kubica-Misztal, A. Korpała, I. Oglodek,
 J. Kowalewski, E. A. Rössler, and J. Moscicki 244502
- Melting behavior of SnI_4 reexamined (7 pages)**
 Kazuhiro Fuchizaki 244503
- First-principles energetics of water clusters and ice: A many-body analysis (9 pages)**
 M. J. Gillan, D. Alfè, A. P. Bartók, and G. Csányi 244504
- Effect of attractive interactions on the water-like anomalies of a core-softened model potential (9 pages)**
 Shashank Pant, Tarun Gera, and Niharendu Choudhury 244505
- Variation and decomposition of the partial molar volume of small gas molecules in different organic solvents derived from molecular dynamics simulations (14 pages)**
 Marco Klähn, Alistair Martin, Daniel W. Cheong, and Marc V. Garland 244506

Surfaces, Interfaces, and Materials

- Elementary steps of the catalytic NO_x reduction with NH_3 : Cluster studies on reaction paths and energetics at vanadium oxide substrate (8 pages)**
 M. Gruber and K. Hermann 244701
- Pressure dependence of Kapitza resistance at gold/water and silicon/water interfaces (10 pages)**
 An Pham, Murat Barisik, and BoHung Kim 244702
- Total reflection infrared spectroscopy of water-ice and frozen aqueous NaCl solutions (8 pages)**
 Rachel L. Walker, Keith Searles, Jesse A. Willard, and Rebecca R. H. Michelsen 244703
- Theoretical modeling of the uranium 4f XPS for U(VI) and U(IV) oxides (13 pages)**
 Paul S. Bagus, Connie J. Nelin, and Eugene S. Ilton 244704
- The thermodynamic properties of hydrated $\gamma\text{-Al}_2\text{O}_3$ nanoparticles (9 pages)**
 Elinor C. Spencer, Baiyu Huang, Stewart F. Parker, Alexander I. Kolesnikov,
 Nancy L. Ross, and Brian F. Woodfield 244705
- Dual passivation of GaAs (110) surfaces using $\text{O}_2/\text{H}_2\text{O}$ and trimethylaluminum (8 pages)**
 Tyler J. Kent, Mary Edmonds, Evgueni Chagarov, Ravi Droopad, and Andrew C. Kummel 244706
- Towards a specific reaction parameter density functional for reactive scattering of H_2 from Pd(111) (11 pages)**
 J. M. Boereboom, M. Wijzenbroek, M. F. Somers, and G. J. Kroes 244707
- Pair correlation functions of two- and three-dimensional hard-core fluids confined into narrow pores: Exact results from transfer-matrix method (6 pages)**
 Péter Gurin and Szabolcs Varga 244708

Polymers and Soft Matter

- Self-assembly of an amphiphilic macromolecule under spherical confinement: An efficient route to generate hollow nanospheres (8 pages)**
 A. A. Glagoleva, V. V. Vasilevskaya, K. Yoshikawa, and A. R. Khokhlov 244901
- Conformational disorder in alkylsiloxane monolayers at elevated temperatures (8 pages)**
 Jan Weber, Thorsten Balgar, and Eckart Hasselbrink 244902

(Continued)

Adsorption of branched and dendritic polymers onto flat surfaces: A Monte Carlo study (11 pages) J.-U. Sommer, J. S. Kłos, and O. N. Mironova	244903
Dynamics of the modulated distortions in confined nematic liquid crystals (6 pages) A. V. Zakharov and A. A. Vakulenko	244904
Stabilization of charged and neutral colloids in salty mixtures (6 pages) Sela Samin and Yoav Tsori	244905
A united event grand canonical Monte Carlo study of partially doped polyaniline (9 pages) M. S. Byshkin, A. Correa, F. Buonocore, A. Di Matteo, and G. Milano	244906
Water dependence of the dielectric β-relaxation in poly(ϵ-caprolactone) (6 pages) B. Kuttich, C. Lederle, and B. Stühn	244907
Electric potential profile of a spherical soft particle with a charged core (5 pages) Anh D. Phan, Dustin A. Tracy, T. L. Hoai Nguyen, N. A. Viet, The-Long Phan, and Thanh H. Nguyen	244908
A self-consistent field study of diblock copolymer/charged particle system morphologies for nanofiltration membranes (14 pages) Bo Zhang, Xianggui Ye, and Brian J. Edwards	244909
Phase diagram of a reentrant gel of patchy particles (12 pages) Sándalo Roldán-Vargas, Frank Smallenburg, Walter Kob, and Francesco Sciortino	244910
Field theoretic simulations of polymer nanocomposites (11 pages) Jason Koski, Huikuan Chao, and Robert A. Riggleman	244911
Revisiting the influence of chain length on the α- and β-relaxations in oligomeric glass formers (6 pages) K. L. Ngai	244912

Biological Molecules and Networks

Non-Markovian properties and multiscale hidden Markovian network buried in single molecule time series (12 pages) Tahmina Sultana, Hiroaki Takagi, Miki Morimatsu, Hiroshi Teramoto, Chun-Biu Li, Yasushi Sako, and Tamiki Komatsuzaki	245101
---	---------------

LETTERS TO THE EDITOR

Errata

Erratum: "Thermodynamic properties of supercritical n-m Lennard-Jones fluids and isochoric and isobaric heat capacity maxima and minima" [J. Chem. Phys. 139, 154503 (2013)] (2 pages) Jonas Mairhofer and Richard J. Sadus	249901
---	---------------