

AIP | The Journal of Chemical Physics



► **Cover image** from Martina Pannuzzo, Antonio Raudino, and Rainer A. Böckmann, *J. Chem. Phys.* **141**, 024901 (2014).

COMMUNICATIONS

Communication: Separable potential energy surfaces from multiplicative artificial neural networks (4 pages)
Werner Koch and Dong H. Zhang 021101

ARTICLES

Theoretical Methods and Algorithms

- Efficient algorithms for semiclassical instanton calculations based on discretized path integrals (14 pages)**
Tsutomu Kawatsu and Shinichi Miura 024101
- Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks (19 pages)**
Dmitry Zuev, Thomas-C. Jagau, Ksenia B. Bravaya, Evgeny Epifanovsky, Yihan Shao, Eric Sundstrom, Martin Head-Gordon, and Anna I. Krylov 024102
- The complex chemical Langevin equation (18 pages)**
David Schnoerr, Guido Sanguinetti, and Ramon Grima 024103
- Fast variance reduction for steady-state simulation and sensitivity analysis of stochastic chemical systems using shadow function estimators (8 pages)**
Andreas Miliias-Argeitis, John Lygeros, and Mustafa Khammash 024104
- Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework (11 pages)**
Daniel Berger, Andrew J. Logsdail, Harald Oberhofer, Matthew R. Farrow, C. Richard A. Catlow, Paul Sherwood, Alexey A. Sokol, Volker Blum, and Karsten Reuter 024105
- New tools for the systematic analysis and visualization of electronic excitations. I. Formalism (13 pages)**
Felix Plasser, Michael Wormit, and Andreas Dreuw 024106
- New tools for the systematic analysis and visualization of electronic excitations. II. Applications (12 pages)**
Felix Plasser, Stefanie A. Bäßler, Michael Wormit, and Andreas Dreuw 024107
- Magnetizability and rotational g tensors for density fitted local second-order Møller-Plesset perturbation theory using gauge-including atomic orbitals (23 pages)**
Stefan Loibl and Martin Schütz 024108
- Bowl breakout: Escaping the positive region when searching for saddle points (7 pages)**
Andreas Pedersen and Mathieu Luisier 024109
- Novel type of chimera spiral waves arising from decoupling of a diffusible component (7 pages)**
Xiaodong Tang, Tao Yang, Irving R. Epstein, Yang Liu, Yuemin Zhao, and Qingyu Gao 024110
- Multipole plasmon excitations of C_{60} dimers (5 pages)**
Afshin Moradi 024111
- Assessment of density functional theory based Δ SCF (self-consistent field) and linear response methods for longest wavelength excited states of extended π -conjugated molecular systems (9 pages)**
Michael Filatov and Miquel Huix-Rotllant 024112

Orbital-dependent second-order scaled-opposite-spin correlation functionals in the optimized effective potential method (12 pages) Ireneusz Grabowski, Eduardo Fabiano, Andrew M. Teale, Szymon Śmiga, Adam Buksztel, and Fabio Della Sala	024113
Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation (13 pages) Qi Ou, Shervin Fatehi, Ethan Alguire, Yihan Shao, and Joseph E. Subotnik	024114
An ionic concentration and size dependent dielectric permittivity Poisson-Boltzmann model for biomolecular solvation studies (8 pages) Hanlin Li and Benzhuo Lu	024115
Ring polymer dynamics for rigid tops with an improved integrator (8 pages) S. Wolf and E. Curotto	024116
Irreversible thermodynamics of open chemical networks. I. Emergent cycles and broken conservation laws (17 pages) Matteo Poletini and Massimiliano Esposito	024117
A MATLAB-based finite-element visualization of quantum reactive scattering. I. Collinear atom-diatom reactions (15 pages) Mick Warehime and Millard H. Alexander	024118
Tensor hypercontracted ppRPA: Reducing the cost of the particle-particle random phase approximation from $O(r^6)$ to $O(r^4)$ (7 pages) Neil Shenvi, Helen van Aggelen, Yang Yang, and Weitao Yang	024119
Advanced Experimental Techniques	
A new broadband homonuclear mixing pulse for NMR with low applied power (6 pages) Paul Coote, Kendra E. Leigh, Tsyr-Yan Yu, Navin Khaneja, Gerhard Wagner, and Haribabu Arthanari	024201
Atoms, Molecules, and Clusters	
Differential cross sections for intermediate-energy electron scattering from α-tetrahydrofurfuryl alcohol: Excitation of electronic-states (8 pages) L. Chiari, H. V. Duque, D. B. Jones, P. A. Thorn, Z. Pettifer, G. B. da Silva, P. Limão-Vieira, D. Dufлот, M.-J. Hubin-Franskin, J. Delwiche, F. Blanco, G. García, M. C. A. Lopes, K. Ratnavelu, R. D. White, and M. J. Brunger	024301
Thermal radiation of laser heated niobium clusters Nb_N^+, $8 \leq N \leq 22$ (7 pages) Klavs Hansen, Yejun Li, Vladimir Kaydashev, and Ewald Janssens	024302
$O_2(b^1\Sigma_g^+, v = 0, 1)$ relative yields in $O(^1D) + O_2$ energy transfer (5 pages) Dušan A. Pejaković, Richard A. Copeland, Tom G. Slanger, and Konstantinos S. Kalogerakis	024303
Rotationally resolved state-to-state photoelectron study of niobium carbide radical (5 pages) Zhihong Luo, Huang Huang, Zheng Zhang, Yih-Chung Chang, and C. Y. Ng	024304
Theoretical oxidation state analysis of Ru-(bpy)₃: Influence of water solvation and Hubbard correction in first-principles calculations (6 pages) Kyle G. Reeves and Yosuke Kanai	024305
Infrared spectroscopy of the acetyl cation and its protonated ketene isomer (7 pages) J. D. Mosley, J. W. Young, and M. A. Duncan	024306
The dependence of homogeneous nucleation rate on supersaturation (7 pages) Steven L. Girshick	024307

(Continued)

- Production of cold beams of ND₃ with variable rotational state distributions by electrostatic extraction of He and Ne buffer-gas-cooled beams (10 pages)**
 Kathryn S. Twyman, Martin T. Bell, Brianna R. Heazlewood, and Timothy P. Softley 024308

Liquids, Glasses, and Crystals

- On the room-temperature phase diagram of high pressure hydrogen: An *ab initio* molecular dynamics perspective and a diffusion Monte Carlo study (9 pages)**
 Ji Chen, Xinguo Ren, Xin-Zheng Li, Dario Alfè, and Enge Wang 024501
- Reversible amorphous-crystalline phase changes in a wide range of Se_{1-x}Te_x alloys studied using ultrafast differential scanning calorimetry (9 pages)**
 Paul. A. Vermeulen, Jamo Momand, and Bart J. Kooi 024502
- An electronic criterion for assessing intrinsic brittleness of metallic glasses (6 pages)**
 X. F. Wang, T. E. Jones, Y. Wu, Z. P. Lu, S. Halas, T. Durakiewicz, and M. E. Eberhart 024503
- Liquid-state polaron theory of the hydrated electron revisited (11 pages)**
 James P. Donley, David R. Heine, Caleb A. Tormey, and David T. Wu 024504
- Lithium hydroxide, LiOH, at elevated densities (11 pages)**
 Andreas Hermann, N. W. Ashcroft, and Roald Hoffmann 024505
- The effect of substrate on thermodynamic and kinetic anisotropies in atomic thin films (15 pages)**
 Amir Haji-Akbari and Pablo G. Debenedetti 024506
- Structural, vibrational, and elastic properties of a calcium aluminosilicate glass from molecular dynamics simulations: The role of the potential (9 pages)**
 M. Bauchy 024507
- Diffusion affected magnetic field effect in exciplex fluorescence (5 pages)**
 Anatoly I. Burshtein and Anatoly I. Ivanov 024508
- Ultrafast pump-probe and 2DIR anisotropy and temperature-dependent dynamics of liquid water within the E3B model (10 pages)**
 Yicun Ni and J. L. Skinner 024509
- Simulating the vibrational spectra of ionic liquid systems: 1-Ethyl-3-methylimidazolium acetate and its mixtures (11 pages)**
 Martin Thomas, Martin Brehm, Oldamur Hollóczki, Zsolt Kelemen, László Nyulászi, Tibor Pasinszki, and Barbara Kirchner 024510
- Critical point of gas-liquid type phase transition and phase equilibrium functions in developed two-component plasma model (6 pages)**
 M. A. Butlitsky, B. B. Zelener, and B. V. Zelener 024511

Surfaces, Interfaces, and Materials

- Dynamics of H₂ Eley-Rideal abstraction from W(110): Sensitivity to the representation of the molecule-surface potential (10 pages)**
 R. Pétuya, P. Larrégaray, C. Crespos, H. F. Busnengo, and A. E. Martínez 024701
- The interaction of organic adsorbate vibrations with substrate lattice waves in methyl-Si(111)-(1 × 1) (11 pages)**
 Ryan D. Brown, Zachary M. Hund, Davide Campi, Leslie E. O'Leary, Nathan S. Lewis, M. Bernasconi, G. Benedek, and S. J. Sibener 024702
- Pressure-driven variations of hydrogen bonding energy in ammonium azide (NH₄N₃): IR absorption and Raman scattering studies (8 pages)**
 Xiaoxin Wu, Fengxian Ma, Chunli Ma, Hang Cui, Zhenxian Liu, Hongyang Zhu, Xiaoli Wang, and Qiliang Cui 024703

(Continued)

Toward tailorable surfaces: A combined theoretical and experimental study of lanthanum niobate layered perovskites (9 pages) Stefania Di Tommaso, Francesco Giannici, Adriana Mossuto Marculescu, Antonino Martorana, Carlo Adamo, and Frédéric Labat	024704
Aris-Taylor dispersion in tubes with dead ends (11 pages) Leonardo Dagdug, Alexander M. Berezhkovskii, and Alexei T. Skvortsov	024705
Dynamic mean field theory for lattice gas models of fluids confined in porous materials: Higher order theory based on the Bethe-Peierls and path probability method approximations (10 pages) John R. Edison and Peter A. Monson	024706
First principles studies of proton conduction in KTaO_3 (6 pages) Sung Gu Kang and David S. Sholl	024707
Adapting SAFT-γ perturbation theory to site-based molecular dynamics simulation. II. Confined fluids and vapor-liquid interfaces (23 pages) Ahmadreza F. Ghobadi and J. Richard Elliott	024708

Polymers and Soft Matter

Peptide-induced membrane curvature in edge-stabilized open bilayers: A theoretical and molecular dynamics study (12 pages) Martina Pannuzzo, Antonio Raudino, and Rainer A. Böckmann	024901
Phase diagram of mixtures of colloids and polymers in the thermal crossover from good to θ solvent (17 pages) Giuseppe D'Adamo, Andrea Pelissetto, and Carlo Pierleoni	024902
Coarse-grained molecular simulations of membrane adhesion domains (5 pages) Nadiv Dharan and Oded Farago	024903
Brownian cluster dynamics with short range patchy interactions: Its application to polymers and step-growth polymerization (16 pages) A. Prabhu, S. B. Babu, J. S. Dolado, and J.-C. Gimel	024904
Brownian dynamics simulations of nanosheet solutions under shear (10 pages) Yueyi Xu and Micah J. Green	024905

Biological Molecules and Networks

Effects of knot type in the folding of topologically complex lattice proteins (10 pages) Miguel A. Soler, Ana Nunes, and Patrícia F. N. Faísca	025101
--	--------

LETTERS TO THE EDITOR

Errata

Erratum: "Liquid-crystal mediated nanoparticle interactions and gel formation" [J. Chem. Phys. 138, 194903 (2013)] (1 page) Jonathan K. Whitmer, Abhijeet A. Joshi, Tyler F. Roberts, and Juan J. de Pablo	029901
Erratum: "The exact molecular wavefunction as a product of an electronic and a nuclear wavefunction" [J. Chem. Phys. 138, 224110 (2013)] (2 pages) Lorenz S. Cederbaum	029902
Publisher's Note: "An exploration of the ozone dimer potential energy surface" [J. Chem. Phys. 140, 244311 (2014)] (1 page) Luis Miguel Azofra, Ibon Alkorta, and Steve Scheiner	029903