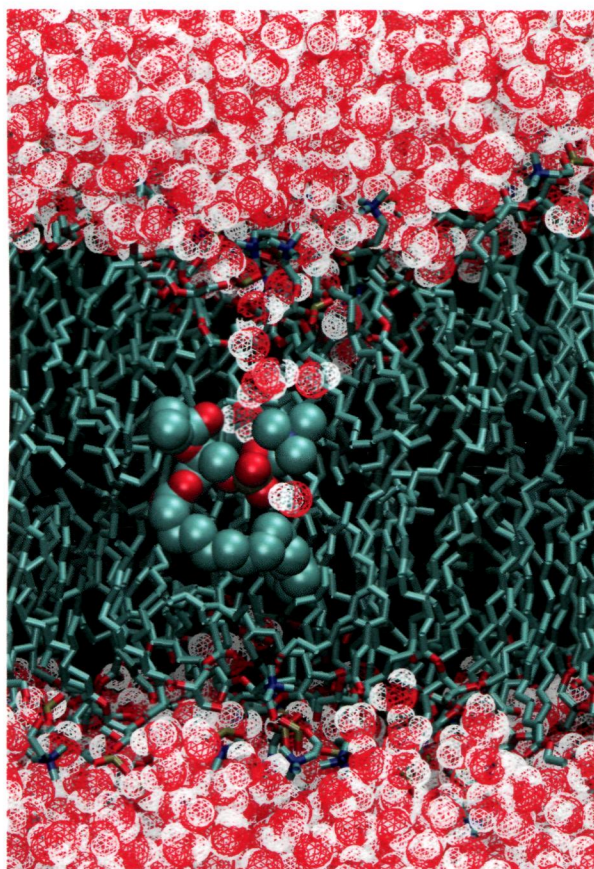


# AIP | The Journal of Chemical Physics



► Cover image from Kun Huang and Angel E. García, *J. Chem. Phys.* **141**, 105101 (2014).

## COMMUNICATIONS

- Communication: High precision sub-Doppler infrared spectroscopy of the HeH<sup>+</sup> ion** (5 pages)  
Adam J. Perry, James N. Hodges, Charles R. Markus, G. Stephen Kocheril,  
and Benjamin J. McCall ..... 101101
- Communication: Coupled-cluster interpretation of the photoelectron spectrum of Au<sub>3</sub><sup>-</sup>** (5 pages)  
Nicholas P. Bauman, Jared A. Hansen, Masahiro Ehara, and Piotr Piecuch ..... 101102
- Communication: Low-temperature approximation of the virial series for the Lennard-Jones  
and modified Lennard-Jones models** (4 pages)  
M. V. Ushcats ..... 101103
- Communication: Supramolecular structures in monohydroxy alcohols: Insights from shear-mechanical  
studies of a systematic series of octanol structural isomers** (5 pages)  
Tina Hecksher and Bo Jakobsen ..... 101104
- Communication: Towards the binding energy and vibrational red shift of the simplest organic  
hydrogen bond: Harmonic constraints for methanol dimer** (4 pages)  
Matthias Heger, Martin A. Suhm, and Ricardo A. Mata ..... 101105

## ARTICLES

### Theoretical Methods and Algorithms

- Plasmons in molecules: Microscopic characterization based on orbital transitions  
and momentum conservation** (11 pages)  
Caroline M. Krauter, Jochen Schirmer, Christoph R. Jacob, Markus Pernpointner,  
and Andreas Dreuw ..... 104101
- Analytic first derivatives for a spin-adapted open-shell coupled cluster theory:  
Evaluation of first-order electrical properties** (12 pages)  
Dipayan Datta and Jürgen Gauss ..... 104102
- Reaction efficiency effects on binary chemical reactions** (4 pages)  
Filippos Lazaridis, Aditya Savara, and Panos Argyrakis ..... 104103
- Analysis of the methods for the derivation of binary kinetic equations in the theory  
of fluorescence concentration quenching** (22 pages)  
A. B. Doktorov ..... 104104
- Efficient anharmonic vibrational spectroscopy for large molecules using local-mode  
coordinates** (16 pages)  
Xiaolu Cheng and Ryan P. Steele ..... 104105
- Testing time-dependent density functional theory with depopulated molecular orbitals  
for predicting electronic excitation energies of valence, Rydberg, and charge-transfer  
states and potential energies near a conical intersection** (8 pages)  
Shaohong L. Li and Donald G. Truhlar ..... 104106

<b>Measuring disorder in irreversible decay processes (5 pages)</b> Shane W. Flynn, Helen C. Zhao, and Jason R. Green .....	104107
<b>On the full exploitation of symmetry in periodic (as well as molecular) self-consistent-field <i>ab initio</i> calculations (9 pages)</b> Roberto Orlando, Marco De La Pierre, Claudio M. Zicovich-Wilson, Alessandro Erba, and Roberto Dovesi .....	104108
<b>Linear and second-order nonlinear optical properties of ionic organic crystals (10 pages)</b> Tomasz Seidler, Katarzyna Stadnicka, and Benoît Champagne .....	104109
<b>Adding flexibility to the “particles-on-a-sphere” model for large-amplitude motion: POSflex force field for protonated methane (12 pages)</b> Felix Uhl, Łukasz Walewski, Harald Forbert, and Dominik Marx .....	104110

### Advanced Experimental Techniques

<b>Towards bio-silicon interfaces: Formation of an ultra-thin self-hydrated artificial membrane composed of dipalmitoylphosphatidylcholine (DPPC) and chitosan deposited in high vacuum from the gas-phase (7 pages)</b> María J. Retamal, Marcelo A. Cisternas, Sebastian E. Gutierrez-Maldonado, Tomas Perez-Acle, Birger Seifert, Mark Busch, Patrick Huber, and Ulrich G. Volkmann .....	104201
<b>Accurate measurement of heteronuclear dipolar couplings by phase-alternating R-symmetry (PARS) sequences in magic angle spinning NMR spectroscopy (11 pages)</b> Guangjin Hou, Xingyu Lu, Alexander J. Vega, and Tatyana Polenova .....	104202

### Atoms, Molecules, and Clusters

<b>A new accurate ground-state potential energy surface of ethylene and predictions for rotational and vibrational energy levels (16 pages)</b> Thibault Delahaye, Andrei Nikitin, Michaël Rey, Péter G. Szalay, and Vladimir G. Tyuterev .....	104301
<b>A systematic approach to vertically excited states of ethylene using configuration interaction and coupled cluster techniques (21 pages)</b> David Feller, Kirk A. Peterson, and Ernest R. Davidson .....	104302
<b>Theoretical spectroscopic characterization at low temperatures of S-methyl thioformate and O-methyl thioformate (10 pages)</b> M. L. Senent, C. Puzzarini, M. Hochlaf, R. Domínguez-Gómez, and M. Carvajal .....	104303
<b>Nanothermodynamics of large iron clusters by means of a flat histogram Monte Carlo method (19 pages)</b> M. Basire, J.-M. Soudan, and C. Angelié .....	104304
<b>Generation and structural characterization of aluminum cyanoacetylide (7 pages)</b> Carlos Cabezas, Carmen Barrientos, Antonio Largo, Jean-Claude Guillemin, José Cernicharo, Isabel Peña, and José L. Alonso .....	104305
<b>A new <i>ab initio</i> potential energy surface and infrared spectra for the Ar-CS<sub>2</sub> complex (6 pages)</b> Ting Yuan, Xueli Sun, Yi Hu, and Hua Zhu .....	104306
<b>Revisiting the photodissociation dynamics of the phenyl radical (9 pages)</b> Neil C. Cole-Filipiak, Mark Shapero, Bogdan Negru, and Daniel M. Neumark .....	104307
<b>Detailed mechanism of the CH<sub>2</sub>I + O<sub>2</sub> reaction: Yield and self-reaction of the simplest Criegee intermediate CH<sub>2</sub>OO (11 pages)</b> Wei-Lun Ting, Chun-Hung Chang, Yu-Fang Lee, Hiroyuki Matsui, Yuan-Pern Lee, and Jim Jr-Min Lin .....	104308

<b>Low energy electron induced cytosine base release in 2'-deoxycytidine-3'-monophosphate via glycosidic bond cleavage: A time-dependent wavepacket study (9 pages)</b> Renjith Bhaskaran and Manabendra Sarma .....	104309
<b>Comparative study of water reactivity with <math>\text{Mo}_2\text{O}_y^-</math> and <math>\text{W}_2\text{O}_y^-</math> clusters: A combined experimental and theoretical investigation (9 pages)</b> Manisha Ray, Sarah E. Waller, Arjun Saha, Krishnan Raghavachari, and Caroline Chick Jarrold .....	104310
<b>Valence and ionic lowest-lying electronic states of ethyl formate as studied by high-resolution vacuum ultraviolet photoabsorption, He(I) photoelectron spectroscopy, and <i>ab initio</i> calculations (9 pages)</b> M. A. Śmiatek, M. Łabuda, J. Guthmuller, M.-J. Hubin-Franskin, J. Delwiche, D. Duflot, N. J. Mason, S. V. Hoffmann, N. C. Jones, and P. Limão-Vieira .....	104311
<b><i>Ab initio</i> potential energy curves of the valence, Rydberg, and ion-pair states of iodine monochloride, ICl (10 pages)</b> Apostolos Kalamos and Rita Prosimiti .....	104312
<b>Vibrational spectra and structures of bare and Xe-tagged cationic <math>\text{Si}_n\text{O}_m^+</math> clusters (9 pages)</b> Marco Savoca, Judith Langer, Dan J. Harding, Dennis Palagin, Karsten Reuter, Otto Dopfer, and André Fielicke .....	104313
<b>A diabatic state model for double proton transfer in hydrogen bonded complexes (6 pages)</b> Ross H. McKenzie .....	104314
<b>Excited states of <math>\text{OH}-(\text{H}_2\text{O})_n</math> clusters for <math>n = 1-4</math>: An <i>ab initio</i> study (9 pages)</b> Gerald J. Hoffman, Pradeep K. Gurunathan, Joseph S. Francisco, and Lyudmila V. Slipchenko .....	104315
<b>Photodissociation dynamics of <math>\text{C}_3\text{H}_5\text{I}</math> in the near-ultraviolet region (8 pages)</b> Masataka Sumida, Takuya Hanada, Katsuyoshi Yamasaki, and Hiroshi Kohguchi .....	104316
<b>Collision dynamics of polyatomic molecules containing carbon rings at low temperatures (8 pages)</b> Zhiying Li, Roman V. Krems, and Eric J. Heller .....	104317
<b>Accurate evaluations of the field shift and lowest-order QED correction for the ground <math>1^1\text{S}</math>-states of some light two-electron ions (10 pages)</b> Alexei M. Frolov and David M. Wardlaw .....	104318
<b>Interaction of toluene with two-color asymmetric laser fields: Controlling the directional emission of molecular hydrogen fragments (7 pages)</b> S. Kaziannis, N. Kotsina, and C. Kosmidis .....	104319
<b>A systematic study of Rayleigh-Brillouin scattering in air, <math>\text{N}_2</math>, and <math>\text{O}_2</math> gases (10 pages)</b> Ziyu Gu and Wim Ubachs .....	104320
<b>Effect of counterions on the charging mechanisms of a macromolecule in aqueous nanodrops (11 pages)</b> Mahmoud Sharawy and Styliani Consta .....	104321
<b>Liquids, Glasses, and Crystals</b>	
<b>Slow solvation in ionic liquids: Connections to non-Gaussian moves and multi-point correlations (12 pages)</b> Tamisra Pal and Ranjit Biswas .....	104501
<b>Quantum fluctuations and isotope effects in <i>ab initio</i> descriptions of water (6 pages)</b> Lu Wang, Michele Ceriotti, and Thomas E. Markland .....	104502
<b>Structure of fluid mixtures near a solute: A density functional approach (7 pages)</b> Chandra N. Patra .....	104503

<b>Simple physics of the partly pinned fluid systems (12 pages)</b> Vincent Krakowiack .....	104504
<b>Equations of state of ice VI and ice VII at high pressure and high temperature (6 pages)</b> Lucile Bezacier, Baptiste Journaux, Jean-Philippe Perrillat, Hervé Cardon, Michael Hanfland, and Isabelle Daniel .....	104505
<b>Comparative study of dynamics in glass forming mixtures of Debye-type N-ethylacetamide with water, alcohol, and amine (9 pages)</b> Xin Li, Zeming Chen, Zijiang Li, Yanqin Gao, Wenkang Tu, Xiangqian Li, Yaqi Zhang, Ying Dan Liu, and Li-Min Wang .....	104506
<b>A scaled-ionic-charge simulation model that reproduces enhanced and suppressed water diffusion in aqueous salt solutions (7 pages)</b> Z. R. Kann and J. L. Skinner .....	104507
<b>Thermal conductivity of halide solid solutions: Measurement and prediction (12 pages)</b> Aïmen E. Gheribi, Sándor Poncsák, Rémi St-Pierre, László I. Kiss, and Patrice Chartrand .....	104508
<b>Diffusional motion of redox centers in carbonate electrolytes (8 pages)</b> Kee Sung Han, Nav Nidhi Rajput, Xiaoliang Wei, Wei Wang, Jian Zhi Hu, Kristin A. Persson, and Karl T. Mueller .....	104509
<b>Effect of physical aging on Johari-Goldstein relaxation in La-based bulk metallic glass (4 pages)</b> Jichao Qiao, Riccardo Casalini, and Jean-Marc Pelletier .....	104510

### Surfaces, Interfaces, and Materials

<b>Water and formic acid aggregates: A molecular dynamics study (8 pages)</b> Delphine Vardanega and Sylvain Picaud .....	104701
<b>Preparation of gallium nitride surfaces for atomic layer deposition of aluminum oxide (9 pages)</b> A. J. Kerr, E. Chagarov, S. Gu, T. Kaufman-Osborn, S. Madiseti, J. Wu, P. M. Asbeck, S. Oktyabrsky, and A. C. Kummel .....	104702
<b>Temperature-dependent infrared dielectric functions of MgO crystal: An ellipsometry and first-principles molecular dynamics study (7 pages)</b> J. Y. Yang, W. J. Zhang, L. H. Liu, J. Qiu, K. Wang, and J. Y. Tan .....	104703
<b>Thermally and photoinduced polymerization of ultrathin sexithiophene films (8 pages)</b> Anke Sander, Rene Hammer, Klaus Duncker, Stefan Förster, and Wolf Widdra .....	104704

### Polymers and Soft Matter

<b>Molecular simulation study of role of polymer-particle interactions in the strain-dependent viscoelasticity of elastomers (Payne effect) (11 pages)</b> Yulong Chen, Ziwei Li, Shipeng Wen, Qingyuan Yang, Liqun Zhang, Chongli Zhong, and Li Liu .....	104901
<b>Excluded volume effects in polymer brushes at moderate chain stretching (7 pages)</b> Dirk Romeis and Michael Lang .....	104902
<b>Capillary wave dynamics of thin liquid polymer films (6 pages)</b> Fan-Yen Lin and Werner Steffen .....	104903
<b>Effect of bound state of water on hydronium ion mobility in hydrated Nafion using molecular dynamics simulations (8 pages)</b> Takuya Mabuchi and Takashi Tokumasu .....	104904
<b>Volume phase transition of polyelectrolyte gels: Effects of ionic size (6 pages)</b> Li-Jian Qu, Xinghua Zhang, Jiuzhou Tang, Lin Li, and Dadong Yan .....	104905

**Ordered structures of small numbers of nanorods induced by semiflexible star polymers (6 pages)**  
 Dong Zhang, Lilin He, and Linxi Zhang ..... 104906

**Local-heterogeneous responses and transient dynamics of cage breaking and formation in colloidal fluids (12 pages)**  
 Preetom Nag, Hiroshi Teramoto, Chun-Biu Li, Joseph Z. Terdik, Norbert F. Scherer, and Tamiki Komatsuzaki ..... 104907

**Polymer brushes in explicit poor solvents studied using a new variant of the bond fluctuation model (10 pages)**  
 Christoph Jentzsch and Jens-Uwe Sommer ..... 104908

**Biological Molecules and Networks**

**Effects of truncating van der Waals interactions in lipid bilayer simulations (9 pages)**  
 Kun Huang and Angel E. García ..... 105101

**A coarse-grained model with implicit salt for RNAs: Predicting 3D structure, stability and salt effect (13 pages)**  
 Ya-Zhou Shi, Feng-Hua Wang, Yuan-Yan Wu, and Zhi-Jie Tan ..... 105102

**Physical origins of the high structural stability of CLN025 with only ten residues (14 pages)**  
 Satoshi Yasuda, Tomohiko Hayashi, and Masahiro Kinoshita ..... 105103

**Potential and flux field landscape theory. II. Non-equilibrium thermodynamics of spatially inhomogeneous stochastic dynamical systems (47 pages)**  
 Wei Wu and Jin Wang ..... 105104

**LETTERS TO THE EDITOR**

**Errata**

**Erratum: "Communication: *Ab initio* study of O<sub>4</sub>H<sup>+</sup>: A tracer molecule in the interstellar medium?" [J. Chem. Phys. 141, 081101 (2014)] (1 page)**  
 George D. Xavier, Margarita I. Bernal-Uruchurtu, and Ramón Hernández-Lamoneda ..... 109901