

JUNE 19, 2014

VOLUME 118

NUMBER 24

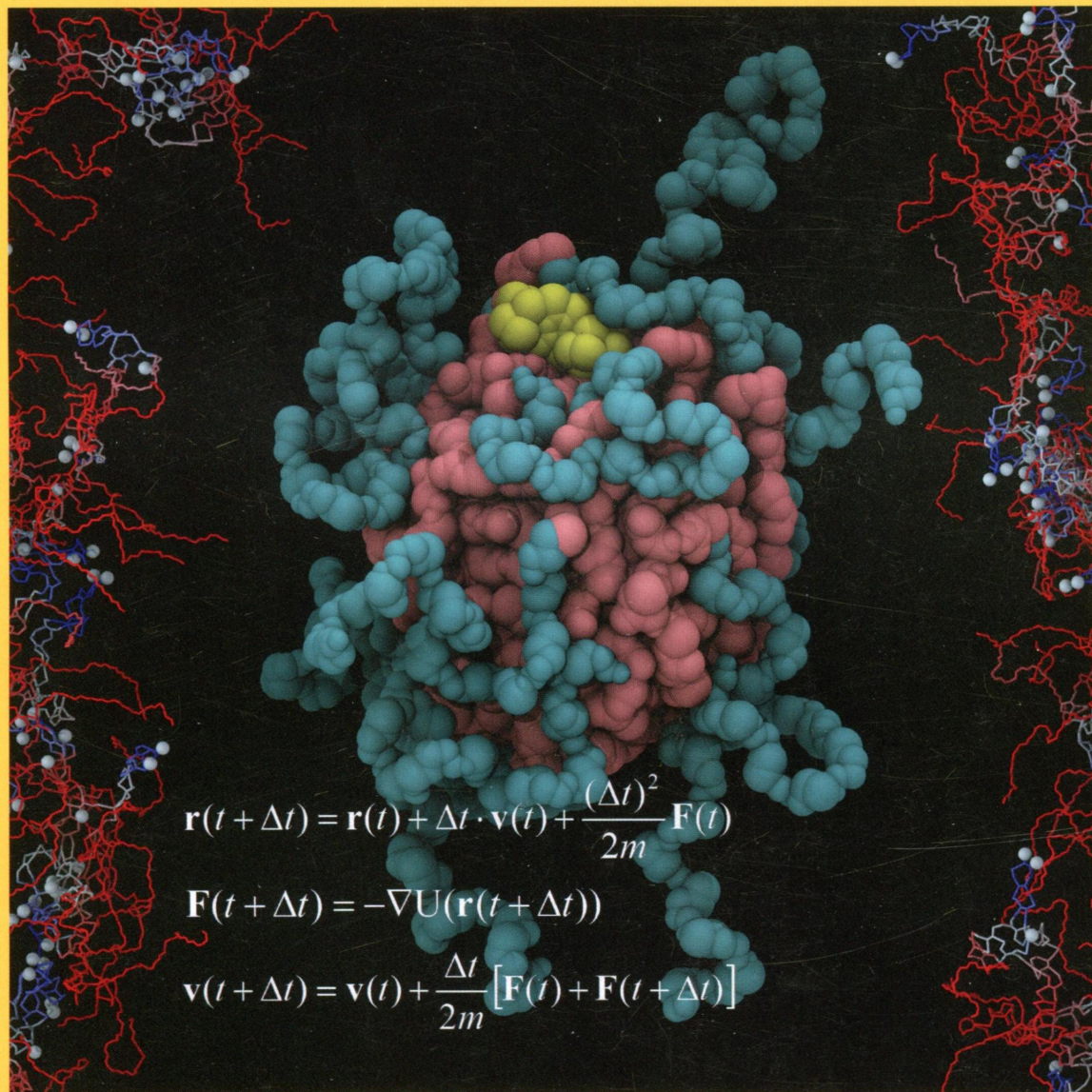
pubs.acs.org/JPCB

THE JOURNAL OF PHYSICAL CHEMISTRY

B

WILLIAM C. SWOPE
FESTSCHRIFT

Molecular Dynamics
Simulations of Drug
Binding to a Star
Polymer, and
Polymer Synthesis



BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

ON THE COVER: Molecular dynamics simulations of drug binding to a star polymer, and polymer synthesis. The cover shows three graphic elements. The equations describe the velocity Verlet algorithm (see: Swope, W. C.; Andersen, H. C.; Berens, P. H.; Wilson, K. R. A. Computer Simulation Method for the Calculation of Equilibrium Constants for the Formation of Physical Clusters of Molecules: Application to Small Water Clusters. *J. Chem. Phys.* **1982**, *76*, 637–649), a standard algorithm for propagating coordinates, and velocities of particles in molecular dynamics programs. The central image is a rendering of a star polymer, which is a polymeric material topologically consisting of several arms chemically bonded to a common molecular framework (core). Each of the sixteen arms on this particular star polymer is a diblock copolymer with a polyester-based hydrophobic region close to the core and a polyethylene glycol (PEG)-based hydrophilic region (blue) farther away (see: Swope, W. C.; Carr, A. C.; Parker, A. J.; Sly, J.; Miller, R. D.; Rice, J. E. Molecular Dynamics Simulations of Star Polymeric Molecules with Diblock Arms, a Comparative Study. *J. Chem. Theory Comput.* **2012**, *8*, 3733–3749). The conformation shown on the cover is from an all atom molecular dynamics simulation of the polymer in explicit water, with the water molecules not shown. In an aqueous environment, the hydrophobic material collapses into a dense layer around the core and the hydrophilic material remains well-solvated. These molecular architectures have been proposed as potential vehicles for the delivery of hydrophobic drug molecules (see Appel, E. A.; Lee, V. Y.; Nguyen, T. T.; McNeil, M.; Nederberg, F.; Hedrick, J. L.; Swope, W. C.; Rice, J. E.; Miller, R. D.; Sly, J. Toward Biodegradable Nanogel Star Polymers via Organocatalytic ROP. *Chem. Commun.* **2012**, *48*, 6163–6165). Near the top is a molecule of ibuprofen, a representative hydrophobic molecule, adsorbed on the star polymer at the water-hydrophobic material interface. This rendering of the van der Waals surface was produced using the VMD (Humphrey, W.; Dalke, A.; Schulten, K. VMD - Visual Molecular Dynamics, *J. Mol. Graphics*, **1996**, *14*, 33–38. <http://www.ks.uiuc.edu/Research/vmd/>) molecular graphics program. Around the edges of the cover image are representative conformations that result from coarse-grained simulations of the synthetic process of polymer formation. The image conveys the temporal order in which regions of the polymer formed, with red indicating material that bonded early and blue indicating material that bonded late during the synthetic process. The white spheres represent functional groups in the polymer, places for further reaction, or potential cargo binding. This part of the figure was also produced using the VMD molecular graphics program. We wish to thank Dr. Amber Carr and Nadine Head-Gordon for effort and ideas related to the cover artwork. This special issue was organized by Guest Editors Teresa Head-Gordon and Julia Rice.

SPECIAL SECTION: WILLIAM C. SWOPE FESTSCHRIFT

Guest Editors: Teresa Head-Gordon and Julia Rice

Special Issue Preface

6357

Tribute to William C. Swope
Teresa Head-Gordon* and Julia Rice

dx.doi.org/10.1021/jp502812z

6360

Personal Observations: William C. Swope
William C. Swope*

dx.doi.org/10.1021/jp502441b

6364

Collaborators of William C. Swope







dx.doi.org/10.1021/jp502438h

6365

Publications of William C. Swope

dx.doi.org/10.1021/jp5024394


Articles

- 6368  [dx.doi.org/10.1021/jp407900c](https://doi.org/10.1021/jp407900c)
The Effects of Flanking Sequences in the Interaction of Polyglutamine Peptides with a Membrane Bilayer
Anu Nagarajan, Sudi Jawahery, and Silvana Matysiak*
- 6380  [dx.doi.org/10.1021/jp410019f](https://doi.org/10.1021/jp410019f)
Multistage Unfolding of an SH3 Domain: An Initial Urea-Filled Dry Molten Globule Precedes a Wet Molten Globule with Non-Native Structure
Amrita Dasgupta, Jayant B. Udgaonkar,* and Payel Das*
- 6393 [dx.doi.org/10.1021/jp410232j](https://doi.org/10.1021/jp410232j)
Molecular Recognition of Metabotropic Glutamate Receptor Type 1 (mGluR1): Synergistic Understanding with Free Energy Perturbation and Linear Response Modeling
Seung-gu Kang, Payel Das, Scott J. McGrane, Alan J. Martin, Tien Huynh, Ajay K. Royyuru, Andrew J. Taylor, Paul G. Jones, and Ruhong Zhou*
- 6405  [dx.doi.org/10.1021/jp410275y](https://doi.org/10.1021/jp410275y)
Comparison of Structure Determination Methods for Intrinsically Disordered Amyloid- β Peptides
K. Aurelia Ball, David E. Wemmer, and Teresa Head-Gordon*
- 6417 [dx.doi.org/10.1021/jp4105823](https://doi.org/10.1021/jp4105823)
Extensive Conformational Heterogeneity within Protein Cores
Gregory R. Bowman* and Phillip L. Geissler
- 6424  [dx.doi.org/10.1021/jp411005x](https://doi.org/10.1021/jp411005x)
Use of Enveloping Distribution Sampling to Evaluate Important Characteristics of Biomolecular Force Fields
Wei Huang, Zhixiong Lin, and Wilfred F. van Gunsteren*
- 6431  [dx.doi.org/10.1021/jp4115139](https://doi.org/10.1021/jp4115139)
Field-SEA: A Model for Computing the Solvation Free Energies of Nonpolar, Polar, and Charged Solutes in Water
Libo Li, Christopher J. Fennell,* and Ken A. Dill
- 6438  [dx.doi.org/10.1021/jp411529h](https://doi.org/10.1021/jp411529h)
A Fixed-Charge Model for Alcohol Polarization in the Condensed Phase, and Its Role in Small Molecule Hydration
Christopher J. Fennell,* Karisa L. Wymer, and David L. Mobley*
- 6447 [dx.doi.org/10.1021/jp411588b](https://doi.org/10.1021/jp411588b)
Correlation as a Determinant of Configurational Entropy in Supramolecular and Protein Systems
Andrew T. Fenley, Benjamin J. Killian, Vladimir Hnizdo,* Adam Fedorowicz, Dan S. Sharp, and Michael K. Gilson*

- 6456  [dx.doi.org/10.1021/jp411671a](https://doi.org/10.1021/jp411671a)
Modeling Organochlorine Compounds and the σ -Hole Effect Using a Polarizable Multipole Force Field
Xiaojiao Mu, Qiantao Wang, Lee-Ping Wang, Stephen D. Fried, Jean-Philip Piquemal, Kevin N. Dalby, and Pengyu Ren*
- 6466  [dx.doi.org/10.1021/jp411770f](https://doi.org/10.1021/jp411770f)
Time Step Rescaling Recovers Continuous-Time Dynamical Properties for Discrete-Time Langevin Integration of Nonequilibrium Systems
David A. Sivak,* John D. Chodera, and Gavin E. Crooks
- 6475 [dx.doi.org/10.1021/jp411822r](https://doi.org/10.1021/jp411822r)
Statistical Model Selection for Markov Models of Biomolecular Dynamics
Robert T. McGibbon, Christian R. Schwantes, and Vijay S. Pande*
- 6482  [dx.doi.org/10.1021/jp412003s](https://doi.org/10.1021/jp412003s)
The Remarkable $[\text{ReH}_5]^{2-}$ Dianion: Molecular Structure and Vibrational Frequencies
Chenyang Li, Jay Agarwal, and Henry F. Schaefer III*
- 6491 [dx.doi.org/10.1021/jp412184h](https://doi.org/10.1021/jp412184h)
Molecular Dynamics Simulations of Linear and Cyclic Amphiphilic Polymers in Aqueous and Organic Environments
Lixin Liu, Sreeja Parameswaran, Arjun Sharma, Scott M. Grayson, Henry S. Ashbaugh, and Steven W. Rick*
- 6498  [dx.doi.org/10.1021/jp412362h](https://doi.org/10.1021/jp412362h)
Fundamental Vibrational Frequencies and Spectroscopic Constants of *cis*- and *trans*-HOCS, HSCO, and Isotopologues via Quartic Force Fields
Ryan C. Fortenberry,* Xinchuan Huang, Michael C. McCarthy, T. Daniel Crawford, and Timothy J. Lee*
- 6511  [dx.doi.org/10.1021/jp412459z](https://doi.org/10.1021/jp412459z)
Filling Up the Heme Pocket Stabilizes Apomyoglobin and Speeds Up Its Folding
J. S. Goodman, S.-H. Chao, T. V. Pogorelov,* and M. Gruebele*
- 6519 [dx.doi.org/10.1021/jp4126478](https://doi.org/10.1021/jp4126478)
Separate Electronic Attenuation Allowing a Spin-Component-Scaled Second-Order Møller–Plesset Theory to Be Effective for Both Thermochemistry and Noncovalent Interactions
Matthew Goldey and Martin Head-Gordon*
- 6526  [dx.doi.org/10.1021/jp412776d](https://doi.org/10.1021/jp412776d)
Expected Distributions of Root-Mean-Square Positional Deviations in Proteins
Jed W. Pitera*

6531  [dx.doi.org/10.1021/jp412808m](https://doi.org/10.1021/jp412808m)
DFT-Derived Reactive Potentials for the Simulation of Activated Processes: the Case of CdTe and CdTe:S
Xiao Liang Hu, Riccardo Ciaglia, Fabio Pietrucci, Grégoire A. Gallet, and Wanda Andreoni*


6539  [dx.doi.org/10.1021/jp500193w](https://doi.org/10.1021/jp500193w)
How Accurately Do Current Force Fields Predict Experimental Peptide Conformations? An Adiabatic Free Energy Dynamics Study
Alexandar T. Tzanov, Michel A. Cuendet, and Mark E. Tuckerman*

6553  [dx.doi.org/10.1021/jp500200b](https://doi.org/10.1021/jp500200b)
Experimental and Computational Studies on the Mechanism of Zwitterionic Ring-Opening Polymerization of δ -Valerolactone with N-Heterocyclic Carbenes
Ashwin K. Acharya, Young A. Chang, Gavin O. Jones, Julia E. Rice, James L. Hedrick, Hans W. Horn,* and Robert M. Waymouth*

6561  [dx.doi.org/10.1021/jp500958r](https://doi.org/10.1021/jp500958r)
Evaluating the Strength of Salt Bridges: A Comparison of Current Biomolecular Force Fields
Karl T. Debiec, Angela M. Gronenborn,* and Lillian T. Chong*


Biophysical Chemistry and Biomolecules

6570 [dx.doi.org/10.1021/jp411459w](https://doi.org/10.1021/jp411459w)
From Nucleobases to Nucleolipids: An ITC Approach on the Thermodynamics of Their Interactions in Aqueous Solutions
Angelos Thanassoulas,* Philippe Barthélemy, Laurence Navailles, and Gilles Sigaud









6586  [dx.doi.org/10.1021/jp412416p](https://doi.org/10.1021/jp412416p)
Why Does Substitution of Thymine by 6-Ethynylpyridone Increase the Thermostability of DNA Double Helices?
Antarip Halder, Ayan Datta,* Dhananjay Bhattacharyya,* and Abhijit Mitra*

6597 [dx.doi.org/10.1021/jp500611f](https://doi.org/10.1021/jp500611f)
Single Molecule Conformational Memory Extraction: P5ab RNA Hairpin
Steve Pressé,* Jack Peterson, Julian Lee, Phillip Elms, Justin L. MacCallum, Susan Marqusee, Carlos Bustamante, and Ken Dill

6604  [dx.doi.org/10.1021/jp500980x](https://doi.org/10.1021/jp500980x)
Mapping the Hydropathy of Amino Acids Based on Their Local Solvation Structure
S. Bonella,* D. Raimondo, E. Milanetti, A. Tramontano, and G. Ciccotti

6614  [dx.doi.org/10.1021/jp501165k](https://doi.org/10.1021/jp501165k)
A Map of Dielectric Heterogeneity in a Membrane Protein: the Hetero-Oligomeric Cytochrome b_6f Complex
S. Saif Hasan, Stanislav D. Zakharov, Adrien Chauvet, Valentyn Stadnytskyi, Sergei Savikhin,* and William A. Cramer*

- 6626  [dx.doi.org/10.1021/jp501277z](https://doi.org/10.1021/jp501277z)
Assessment of the Europium(III) Binding Sites on Albumin Using Fluorescence Spectroscopy
Tatiana N. Tikhonova, Evgeny A. Shirshin,* Gleb S. Budylin, Victor V. Fadeev, and Galina P. Petrova
- 6634  [dx.doi.org/10.1021/jp503339g](https://doi.org/10.1021/jp503339g)
Molecular Organization of Cytochrome c_2 near the Binding Domain of Cytochrome bc_1 Studied by Electron Spin–Lattice Relaxation Enhancement
Rafal Pietras, Marcin Sarewicz, and Artur Osyczka*
- 6644  [dx.doi.org/10.1021/jp501503x](https://doi.org/10.1021/jp501503x)
Self-Assembly of Cyclo-diphenylalanine Peptides in Vacuum
Joohyun Jeon and M. Scott Shell*
- 6653  [dx.doi.org/10.1021/jp501624y](https://doi.org/10.1021/jp501624y)
Multiple Stimuli-Switchable Bioelectrocatalysis under Physiological Conditions Based on Copolymer Films with Entrapped Enzyme
Peng Wang, Shuang Liu, and Hongyun Liu*
- 6662  [dx.doi.org/10.1021/jp501879s](https://doi.org/10.1021/jp501879s)
Free Energy Landscape of Lysozyme: Multiple Near-Native Conformational States and Rollover in the Urea Dependence of Folding Energy
U. Mahammad Yasin, Pulikallu Sashi, and Abani K. Bhuyan*
- 6670 [dx.doi.org/10.1021/jp502609b](https://doi.org/10.1021/jp502609b)
Experimental and Solid-State Computational Study of Structural and Dynamic Properties in the Equilibrium Form of Temazepam
Aleksandra Pajzderska,* Kacper Drużbicki, Miguel A. Gonzalez, Jacek Jencyk, Barbara Peplińska, Marcin Jarek, Jadwiga Mielcarek, and Jan Wąsicki
- 6680  [dx.doi.org/10.1021/jp502724w](https://doi.org/10.1021/jp502724w)
Aluminum Interaction with Glutamate and α -Ketoglutarate: A Computational Study
J. I. Mujika,* J. M. Ugalde, and X. Lopez
- 6687  [dx.doi.org/10.1021/jp5030685](https://doi.org/10.1021/jp5030685)
Role of S-turn2 in the Structure, Dynamics, and Function of Mitochondrial Ribosomal A-Site. A Bioinformatics and Molecular Dynamics Simulation Study
Joanna Panecka, Marek Havrila, Kamila Réblová, Jiří Šponer,* and Joanna Trylska*

- 6702  [dx.doi.org/10.1021/jp5030872](https://doi.org/10.1021/jp5030872)
In Situ Analysis of Bacterial Extracellular Polymeric Substances from a *Pseudomonas fluorescens* Biofilm by Combined Vibrational and Single Molecule Force Spectroscopies
Ahmad Fahs, Fabienne Quiles, Dima Jamal, François Humbert, and Grégory Francius*
- 6714  [dx.doi.org/10.1021/jp503185n](https://doi.org/10.1021/jp503185n)
Mapping Single Molecular Binding Kinetics of Carbohydrate-Binding Module with Crystalline Cellulose by Atomic Force Microscopy Recognition Imaging
Mengmeng Zhang, Bin Wang, and Bingqian Xu*
- 6721  [dx.doi.org/10.1021/jp503422c](https://doi.org/10.1021/jp503422c)
Putative Hydrogen Bond to Tyrosine M208 in Photosynthetic Reaction Centers from *Rhodobacter capsulatus* Significantly Slows Primary Charge Separation
Miguel Saggiu, Brett Carter, Xiaoxue Zhou, Kaitlyn Faries, Lynette Cegelski, Dewey Holten, Steven G. Boxer, and Christine Kirmaier*
- 6733  [dx.doi.org/10.1021/jp503458w](https://doi.org/10.1021/jp503458w)
Interactions of a Water-Soluble Fullerene Derivative with Amyloid- β Protofibrils: Dynamics, Binding Mechanism, and the Resulting Salt-Bridge Disruption
Xiaoying Zhou, Wenhui Xi, Yin Luo, Siqin Cao, and Guanghong Wei*
- 6742  [dx.doi.org/10.1021/jp503469s](https://doi.org/10.1021/jp503469s)
Balancing the Interactions of Ions, Water, and DNA in the Drude Polarizable Force Field
Alexey Savelyev and Alexander D. MacKerell Jr.*
- 6758  [dx.doi.org/10.1021/jp503565e](https://doi.org/10.1021/jp503565e)
Polarization Dependence of Aragonite Calcium L-Edge XANES Spectrum Indicates *c* and *b* Axes Orientation
Rebecca A. Metzler* and Peter Rez
- 6767  [dx.doi.org/10.1021/jp503874z](https://doi.org/10.1021/jp503874z)
Raman Optical Activity of a Cyclic Dipeptide Analyzed by Quantum Chemical Calculations Combined with Molecular Dynamics Simulations
Hiroyasu Urago, Torao Suga, Taiki Hirata, Hiroaki Kodama, and Masashi Unno*
- 6775  [dx.doi.org/10.1021/jp504057u](https://doi.org/10.1021/jp504057u)
Majority and Minority Gates Realized in Enzyme-Biocatalyzed Systems Integrated with Logic Networks and Interfaced with Bioelectronic Systems
Shay Mailloux, Natalia Guz, Andrey Zakharchenko, Sergiy Minko, and Evgeny Katz*

Biomaterials, Surfactants, and Membranes

6785

[dx.doi.org/10.1021/jp501374r](https://doi.org/10.1021/jp501374r)

Absence of Schroeder's Paradox in a Nanostructured Block Copolymer Electrolyte Membrane

Keith M. Beers, Sergey Yakovlev, Andrew Jackson, Xin Wang, Alexander Hexemer, Kenneth H. Downing, and Nitash P. Balsara*

6792



[dx.doi.org/10.1021/jp501755k](https://doi.org/10.1021/jp501755k)

Free Energy of PAMAM Dendrimer Adsorption onto Model Biological Membranes

Yongbin Kim, Yongkyu Kwak, and Rakwo Chang*

6803



[dx.doi.org/10.1021/jp5032898](https://doi.org/10.1021/jp5032898)

Salicylamide Cocrystals: Screening, Crystal Structure, Sublimation Thermodynamics, Dissolution, and Solid-State DFT Calculations

Alex N. Manin, Alexander P. Voronin, Nikolay G. Manin, Mikhail V. Vener, Anastasia V. Shishkina, Anatoly S. Lermontov, and German L. Perlovich*

Liquids; Chemical and Dynamical Processes in Solution

6815



[dx.doi.org/10.1021/jp411358d](https://doi.org/10.1021/jp411358d)

Ultrafast Dynamics and Computational Studies on Diaminodicyanoquinodimethanes (DADQs)

Marek Szablewski,* Mark A. Fox, Fernando B. Dias, Hannah Namih, Edward W. Snedden, Simon M. King, DeChang Dai, and Lars-Olof Pålsson*

6829

[dx.doi.org/10.1021/jp5012044](https://doi.org/10.1021/jp5012044)

Carbon Dioxide Solubility in 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide in a Wide Range of Temperatures and Pressures

Javid Safarov,* Rena Hamidova, Martin Stephan, Ismail Kul, Astan Shahverdiyev, and Egon Hassel

6839



[dx.doi.org/10.1021/jp501220v](https://doi.org/10.1021/jp501220v)

Aggregation of a Dibenzo[*b,def*]chrysene Based Organic Photovoltaic Material in Solution

Alexandr N. Simonov,* Peter Kemppinen, Cristina Pozo-Gonzalo, John F. Boas, Ante Bilic, Andrew D. Scully, Adel Attia, Ayman Nafady, Elena A. Mashkina, Kevin N. Winzenberg, Scott E. Watkins,* and Alan M. Bond*

6850



[dx.doi.org/10.1021/jp5012389](https://doi.org/10.1021/jp5012389)

Photoemission Spectra and Density Functional Theory Calculations of 3d Transition Metal–Aqua Complexes (Ti–Cu) in Aqueous Solution

Diana Yepes, Robert Seidel, Bernd Winter,* Jochen Blumberger,* and Pablo Jaque*

6864



[dx.doi.org/10.1021/jp501648x](https://doi.org/10.1021/jp501648x)

Determination of Size of Molecular Clusters of Ethanol by Means of NMR Diffusometry and Hydrodynamic Calculations

Mária Soltésiová, Ladislav Benda, Mikuláš Peksa, Jiří Czernek, and Jan Lang*

6875

[dx.doi.org/10.1021/jp5027459](https://doi.org/10.1021/jp5027459)

A Nucleation-Based Method to Study Hydrophobic Interactions under Confinement: Enhanced Hydrophobic Association Driven by Energetic Contributions

Hyunmi Kim, Samuel J. Keasler, and Bin Chen*

6885

[dx.doi.org/10.1021/jp502968u](https://doi.org/10.1021/jp502968u)

Structure and Aggregation in the 1,3-Dialkyl-imidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid Family: 2. From Single to Double Long Alkyl Side Chains

Carlos E. S. Bernardes, Karina Shimizu, Ana I. M. C. Lobo Ferreira, Luís M. N. B. F. Santos, and José N. Canongia Lopes*

6896

[dx.doi.org/10.1021/jp502995k](https://doi.org/10.1021/jp502995k)

The Dynamic Process of Atmospheric Water Sorption in [BMIM][Ac]: Quantifying Bulk versus Surface Sorption and Utilizing Atmospheric Water as a Structure Probe

Yu Chen, Yuanyuan Cao, Chuanyu Yan, Yuwei Zhang, and Tiancheng Mu*

6908

[dx.doi.org/10.1021/jp5034917](https://doi.org/10.1021/jp5034917)

Graphene Sculpture Nanopores for DNA Nucleobase Sensing

Hatef Sadeghi, L. Algaragholi, T. Pope, S. Bailey, D. Visontai, D. Manrique, J. Ferrer, V. Garcia-Suarez, Sara Sangtarash, and Colin J Lambert*

6915

[dx.doi.org/10.1021/jp5051047](https://doi.org/10.1021/jp5051047)

Structural Rearrangement Accompanying the Ultrafast Electrocyclization Reaction of a Photochromic Molecular Switch

Emanuele Pontecorvo, Carino Ferrante, Christopher G. Elles,* and Tullio Scopigno*

Glasses, Colloids, Polymers, and Soft Matter

6922

[dx.doi.org/10.1021/jp500355n](https://doi.org/10.1021/jp500355n)

Interaction between Hydrophobically Modified 2-Hydroxyethyl Cellulose and Sodium Dodecyl Sulfate Studied by Viscometry and Two-Dimensional NOE NMR Spectroscopy

Jen-Ting Lo, Hsiao-Ting Yen, Chih-Chang Tsai, Bing-Hung Chen,* and Sheng-Shu Hou

6931

[dx.doi.org/10.1021/jp500824e](https://doi.org/10.1021/jp500824e)

Influence of Belousov–Zhabotinsky Substrate Concentrations on Autonomous Oscillation of Polymer Chains with Fe(bpy)₃ Catalyst

Yusuke Hara,* Hiroyuki Mayama, and Kenji Fujimoto

6937

[dx.doi.org/10.1021/jp502178d](https://doi.org/10.1021/jp502178d)

Arrangement of Fibril Side Chains Studied by Molecular Dynamics and Simulated Infrared and Vibrational Circular Dichroism Spectra

Jifí Kessler, Timothy A. Keiderling,* and Petr Bouř*

6946 

[dx.doi.org/10.1021/jp502486a](https://doi.org/10.1021/jp502486a)

Influence of Surface Concentration on Poly(vinyl alcohol) Behavior at the Water–Vacuum Interface: A Molecular Dynamics Simulation Study


Giulio Tesei, Gaio Paradossi, and Ester Chiessi*

6956

[dx.doi.org/10.1021/jp503473u](https://doi.org/10.1021/jp503473u)

Differences in Cationic and Anionic Charge Densities Dictate Zwitterionic Associations and Stimuli Responses

Qing Shao, Luo Mi, Xia Han, Tao Bai, Sijun Liu, Yuting Li, and Shaoyi Jiang*

6963 

[dx.doi.org/10.1021/jp504049r](https://doi.org/10.1021/jp504049r)

Phase Behavior Under a Noncentrosymmetric Interaction: Shifted-Charge Colloids Investigated by Monte Carlo Simulation

Luis E. Sánchez-Díaz, Chwen-Yang Shew,* Xin Li, Bin Wu, Gregory S. Smith, and Wei-Ren Chen*

6972

[dx.doi.org/10.1021/jp5045783](https://doi.org/10.1021/jp5045783)

Confinement Effects on the Dynamic Behavior of Poly(D,L-lactic Acid) upon Incorporation in α -Cyclodextrin

M. T. Viciosa, N. M. Alves, T. Oliveira, M. Dionísio,* and J. F. Mano