

DECEMBER 5, 2013

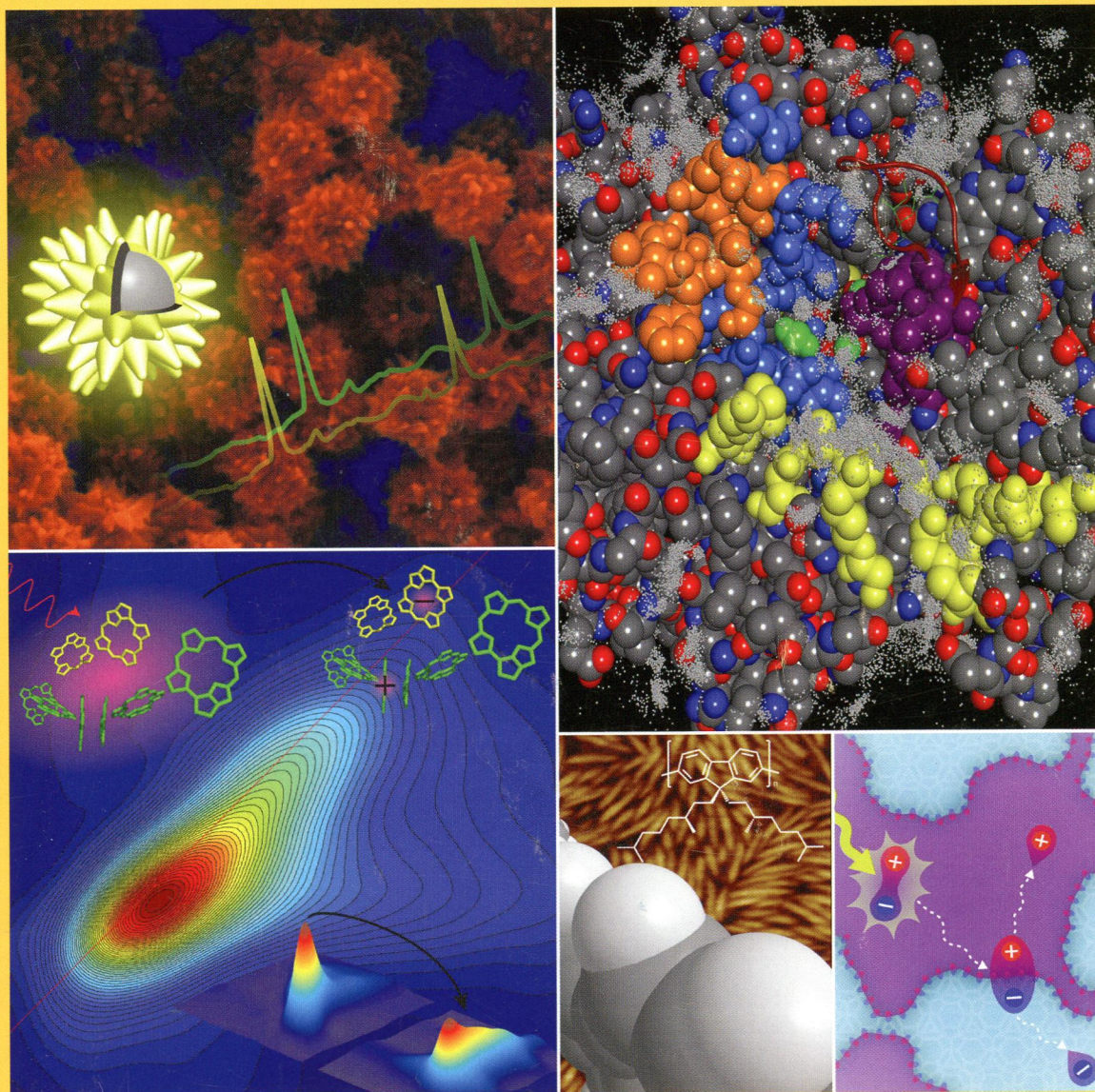
VOLUME 117

NUMBER 48

pubs.acs.org/JPCB

# THE JOURNAL OF PHYSICAL CHEMISTRY

B



**BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER**



**ACS Publications**  
MOST TRUSTED. MOST CITED. MOST READ.

[www.acs.org](http://www.acs.org)



December 5, 2013  
Volume 117, Issue 48  
Pages 14885-15234

***Biophysical Chemistry and Biomolecules***

***Development of an Effective Polarizable Bond Method for Biomolecular Simulation***

Xudong Xiao, Tong Zhu, Chang G. Ji, and John Z. H. Zhang  
pp 14885–14893

**Publication Date (Web):** November 19, 2013 (Article)

**DOI:** 10.1021/jp4080866

 Section:

Biochemical Methods

***Dynamic Nuclear Polarization of  $^{17}\text{O}$ : Direct Polarization***

Vladimir K. Michaelis, Björn Corzilius, Albert A. Smith, and Robert G. Griffin  
pp 14894–14906

**Publication Date (Web):** November 6, 2013 (Article)

**DOI:** 10.1021/jp408440z

 Section:

Magnetic Phenomena

***Changes to the Structure and Dynamics in Mutations of  $\text{A}\beta_{21-30}$  Caused by Ions in Solution***

Micholas Dean Smith and Luis Cruz  
pp 14907–14915

**Publication Date (Web):** November 8, 2013 (Article)

**DOI:** 10.1021/jp408579v

 Section:

General Biochemistry

***Exploring the Dynamic Behaviors and Transport Properties of Gas Molecules in a Transmembrane Cyclic Peptide Nanotube***

Rui Li, Jianfen Fan, Hui Li, Xiliang Yan, and Yi Yu  
pp 14916–14927

**Publication Date (Web):** November 18, 2013 (Article)

**DOI:** 10.1021/jp408769u

 Section:

General Biochemistry

***Networked Enzymatic Logic Gates with Filtering: New Theoretical Modeling Expressions and Their Experimental Application***

Vladimir Privman, Oleksandr Zavalov, Lenka Halámková, Fiona Moseley, Jan Halánek, and Evgeny Katz  
pp 14928–14939

**Publication Date (Web):** November 8, 2013 (Article)

**DOI:** 10.1021/jp408973g

 Section:

Biochemical Methods

### ***Pigment–Protein Interactions in Phytochromes Probed by Fluorescence Line Narrowing Spectroscopy***

Jana B. Nieder, Emina A. Stojković, Keith Moffat, Katrina T. Forest, Tilman Lamparter, Robert Bittl, and John T. M. Kennis

pp 14940–14950

**Publication Date (Web):** November 8, 2013 (Article)

**DOI:** 10.1021/jp409110q

 Section:

General Biochemistry

### ***The Role of Different Structural Motifs in the Ultrafast Dynamics of Second Generation Protein Stains***

Soumit Chatterjee, Peter Karuso, Agathe Boulangé, Philippe A. Peixoto, Xavier Franck, and Anindya Datta

pp 14951–14959

**Publication Date (Web):** October 29, 2013 (Article)

**DOI:** 10.1021/jp4092927

 ACS AuthorChoice

 Section:

Biochemical Methods

### ***Quantum Mechanics/Molecular Mechanics Restrained Electrostatic Potential Fitting***

Steven K. Burger, Jeremy Schofield, and Paul W. Ayers

pp 14960–14966

**Publication Date (Web):** October 31, 2013 (Article)

**DOI:** 10.1021/jp409568h

 Section:

General Biochemistry

### ***Use of Creatine Kinase To Induce Multistep Reactions in Infrared Spectroscopic Experiments***

Nadejda Eremina and Andreas Barth

pp 14967–14972

**Publication Date (Web):** November 14, 2013 (Article)

**DOI:** 10.1021/jp409599p

 Section:

Enzymes

### ***Quantum Mechanics-Based Scoring Rationalizes the Irreversible Inactivation of Parasitic Schistosoma mansoni Cysteine Peptidase by Vinyl Sulfone Inhibitors***

Jindřich Fanfrlík, Pathik S Brahmshatriya, Jan Řezáč, Adéla Jílková, Martin Horn, Michael Mareš, Pavel Hobza, and Martin Lepšík

pp 14973–14982

**Publication Date (Web):** November 6, 2013 (Article)

**DOI:** 10.1021/jp409604n

 Section:

Enzymes

***Lipid Membrane Association of Myelin Proteins and Peptide Segments Studied by Oriented and Synchrotron Radiation Circular Dichroism Spectroscopy***

Gopinath Muruganandam, Jochen Bürck, Anne S. Ulrich, Inari Kursula, and Petri Kursula  
pp 14983–14993

**Publication Date (Web):** November 15, 2013 (Article)

**DOI:** 10.1021/jp4098588

 Section:

General Biochemistry

***Conformational Dynamics of an ATP-Binding DNA Aptamer: A Single-Molecule Study***

Tie Xia, Jinghe Yuan, and Xiaohong Fang

pp 14994–15003

**Publication Date (Web):** November 18, 2013 (Article)

**DOI:** 10.1021/jp4099667

 Section:

General Biochemistry

***Does the Reconstitution of RC-LH1 Complexes from Rhodospseudomonas acidophila Strain 10050 into a Phospholipid Bilayer Yield the Optimum Environment for Optical Spectroscopy?***

Paul S. Böhm, Ralf Kunz, June Southall, Richard J. Cogdell, and Jürgen Köhler

pp 15004–15013

**Publication Date (Web):** November 13, 2013 (Article)

**DOI:** 10.1021/jp409980k

 Section:

Plant Biochemistry

***Biomaterials, Surfactants, and Membranes***

***Aggregation of Double-Tailed Ionic Liquid 1,3-Dioctylimidazolium Bromide and the Interaction with Triblock Copolymer F127***

Lingling Ge, Qi Wang, Duo Wei, Xiaohong Zhang, and Rong Guo

pp 15014–15022

**Publication Date (Web):** November 14, 2013 (Article)

**DOI:** 10.1021/jp405838v

 Section:

Surface Chemistry and Colloids

***Structural Effects of the  $\beta$ -Vinyl Linker in Pyridinium Porphyrins: Spectroscopic Studies in Organic Solvents and AOT Reverse Micelles***

Vanda Vaz Serra, Suzana M. Andrade, Eduarda M. P. Silva, Artur M. S. Silva, Maria G. P. M. S. Neves, and Sílvia M. B. Costa  
pp 15023–15032

**Publication Date (Web):** October 31, 2013 (Article)

**DOI:** 10.1021/jp4076993

 Section:

Physical Organic Chemistry

### ***Octaoctyl-Substituted Lutetium Bisphthalocyanine for NADH Biosensing***

C. Pal, A. K. Sharma, A. N. Cammidge, M. J. Cook, and A. K. Ray

pp 15033–15040

**Publication Date (Web):** November 8, 2013 (Article)

**DOI:** 10.1021/jp4078568

 Section:

Biochemical Methods

### ***Lipid Flip-Flop in Binary Membranes Composed of Phosphatidylserine and Phosphatidylcholine***

Krystal L. Brown and John C. Conboy

pp 15041–15050

**Publication Date (Web):** November 7, 2013 (Article)

**DOI:** 10.1021/jp409672q

 Section:

General Biochemistry

### ***Liquids; Chemical and Dynamical Processes in Solution***

### ***Physicochemical Properties of Tri-n-butylalkylphosphonium Cation-Based Room-Temperature Ionic Liquids***

Kazuki Yoshii, Keisuke Yamaji, Tetsuya Tsuda, Katsuhiko Tsunashima, Hiroyuki Yoshida, Masanori Ozaki, and Susumu Kuwabata

pp 15051–15059

**Publication Date (Web):** November 18, 2013 (Article)

**DOI:** 10.1021/jp406791a

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

### ***Dynamics in the Isotropic Phase of Nematogens Using 2D IR Vibrational Echo Measurements on Natural-Abundance <sup>13</sup>CN and Extended Lifetime Probes***

Kathleen P. Sokolowsky and Michael D. Fayer

pp 15060–15071

**Publication Date (Web):** October 24, 2013 (Article)

**DOI:** 10.1021/jp4071955

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

### ***Phase Diagrams and Solvate Structures of Binary Mixtures of Glymes and Na Salts***



Toshihiko Mandai, Risa Nozawa, Seiji Tsuzuki, Kazuki Yoshida, Kazuhide Ueno, Kaoru Dokko, and Masayoshi Watanabe  
pp 15072–15085

**Publication Date (Web):** November 15, 2013 (Article)

**DOI:** 10.1021/jp407582m

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

### ***Base Triggered Enhancement of First Hyperpolarizability of a Keto–Enol Tautomer***

Soumi De, Manisha Ray, Anusooya Y. Pati, and Puspendu K. Das  
pp 15086–15092

**Publication Date (Web):** November 13, 2013 (Article)

**DOI:** 10.1021/jp410368z

 Section:

Physical Organic Chemistry

### ***Simulations of Acid Dissociation Constants of Polyprotic Acids in Near-Critical and Supercritical Water***

Simon J. Halstead and Pengna An

pp 15093–15100

**Publication Date (Web):** November 14, 2013 (Article)

**DOI:** 10.1021/jp4078932

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

### ***Water Dynamics in Aqueous Solutions of Tetra-n-alkylammonium Salts: Hydrophobic and Coulomb Interactions Disentangled***

Sietse T. van der Post, Stefan Scheidelaar, and Huib J. Bakker

pp 15101–15110

**Publication Date (Web):** November 14, 2013 (Article)

**DOI:** 10.1021/jp4085734

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

### ***Multiregion Shear Thinning for Subsequent Static Self-Thickening in Chitosan-graft-polyacrylamide Aqueous Solution***

Lei Jin, Ye qiang Tan, Yonggang Shangguan, Yu Lin, Bo Xu, Qiang Wu, and Qiang Zheng

pp 15111–15121

**Publication Date (Web):** November 15, 2013 (Article)

**DOI:** 10.1021/jp408782e

 Section:

Physical Properties of Synthetic High Polymers

### ***Measurement of the Relative Mobility of Geminate Ions in Ethereal Solutions of Aromatic Compounds Using the Fluorescence Response of the Solutions to Pulsed Irradiation***

V. I. Borovkov and I. S. Ivanishko

pp 15122–15130

**Publication Date (Web):** November 22, 2013 (Article)

**DOI:** 10.1021/jp4093942

 Section:

Organic Analytical Chemistry

### ***Separation of Carbon Dioxide from Nitrogen or Methane by Supported Ionic Liquid Membranes (SILMs): Influence of the Cation Charge of the Ionic Liquid***

Sandra D. Hojniak, Asim Laeeq Khan, Oldamur Hollóczy, Barbara Kirchner, Ivo F. J. Vankelecom, Wim Dehaen, and Koen Binnemans

pp 15131–15140

**Publication Date (Web):** November 7, 2013 (Article)

**DOI:** 10.1021/jp409414t

 Section:

Unit Operations and Processes

### ***Influence of Acoustic Cavitation on the Controlled Ultrasonic Dispersion of Carbon Nanotubes***

Achilleas Sesis, Mark Hodnett, Gianluca Memoli, Andrew J. Wain, Izabela Jurewicz, Alan B. Dalton, J. David Carey, and Gareth Hinds

pp 15141–15150

**Publication Date (Web):** November 19, 2013 (Article)

**DOI:** 10.1021/jp410041y

 Section:

Ceramics

### ***Erbium(III) in Aqueous Solution: An Ab Initio Molecular Dynamics Study***

Lorenz R. Canaval, Theerathad Sakwarathorn, and Bernd M. Rode, Christoph B. Messner, Oliver M. D. Lutz, and Günther K. Bonn

pp 15151–15156

**Publication Date (Web):** November 19, 2013 (Article)

**DOI:** 10.1021/jp410284z

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

### ***Glasses, Colloids, Polymers, and Soft Matter***

### ***Molecular Dynamics Simulations of the Protonated G4 PAMAM Dendrimer in an Ionic Liquid System***

Juan J. Freire, Amirhossein Ahmadi, and Carl McBride

pp 15157–15164

**Publication Date (Web):** November 14, 2013 (Article)

**DOI:** 10.1021/jp402586s

 Section:

Physical Properties of Synthetic High Polymers

### ***Kinetic and Structural Features of a Dyestuff Coaggregation Studied by Time-Resolved Static Light Scattering***

Rolf Michels, Yvonne Hertle, Thomas Hellweg, and Klaus Huber

pp 15165–15175

**Publication Date (Web):** October 31, 2013 (Article)

**DOI:** 10.1021/jp405206p

 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

### ***Structure and Dynamics of [PF<sub>6</sub>][P<sub>1,2,2,4</sub>] from Molecular Dynamics Simulations***

Marcelo A. Carignano

pp 15176–15183

**Publication Date (Web):** November 21, 2013 (Article)

**DOI:** 10.1021/jp407648b

 Section:

Crystallography and Liquid Crystals

### ***Li Diffusion and the Effect of Local Structure on Li Mobility in Li<sub>2</sub>O–SiO<sub>2</sub> Glasses***

Ute Bauer, Anna-Maria Welsch, Harald Behrens, Johanna Rahn, Harald Schmidt, and Ingo Horn

pp 15184–15195

**Publication Date (Web):** November 6, 2013 (Article)

**DOI:** 10.1021/jp408805e

 Section:

Electric Phenomena

### ***Effect of Aging the Glass of Isotactic Polybutene-1 on Form II Nucleation and Cold Crystallization***

Isabell Stolte, René Androsch, Maria Laura Di Lorenzo, and Christoph Schick

pp 15196–15203

**Publication Date (Web):** November 11, 2013 (Article)

**DOI:** 10.1021/jp4093404

 Section:

Physical Properties of Synthetic High Polymers

### ***Microscopically Based Calculations of the Free Energy Barrier and Dynamic Length Scale in Supercooled Liquids: The Comparative Role of Configurational Entropy and Elasticity***

Pyotr Rabochiy, Peter G. Wolynes, and Vassiliy Lubchenko

pp 15204–15219

**Publication Date (Web):** November 6, 2013 (Article)

**DOI:** 10.1021/jp409502k

 Section:

General Physical Chemistry

### ***Optical Spectra and Band Structure of Ag<sub>x</sub>Ga<sub>x</sub>Ge<sub>1-x</sub>Se<sub>2</sub> (x = 0.333, 0.250, 0.200, 0.167) Single Crystals: Experiment and Theory***

A. H. Reshak, O. V. Parasyuk, A. O. Fedorchuk, H. Kamarudin, S. Auluck, and J. Chyský

pp 15220–15231

**Publication Date (Web):** November 12, 2013 (Article)

**DOI:** 10.1021/jp410786w



 Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

### ***Additions and Corrections***

#### ***Correction to “Characterization of Supported Lipid Bilayer Disruption by Chrysoepsin-3 Using QCM-D”***

Kathleen F. Wang, Ramanathan Nagarajan, Charlene M. Mello, and Terri A. Camesano

pp 15232–15232

**Publication Date (Web):** November 20, 2013 (Addition/Correction)

**DOI:** 10.1021/jp410498b

 Section:

General Biochemistry

#### ***Correction to “Transient Helical Structure during PI3K and Fyn SH3 Domain Folding”***

Yoshitaka Matsumura, Masaji Shinjo, Seung Joong Kim, Nobuyuki Okishio, Martin Gruebele, and Hiroshi Kihara

pp 15233–15233

**Publication Date (Web):** November 22, 2013 (Addition/Correction)

**DOI:** 10.1021/jp411258t

 Section:

General Biochemistry