

JUNE 6, 2013

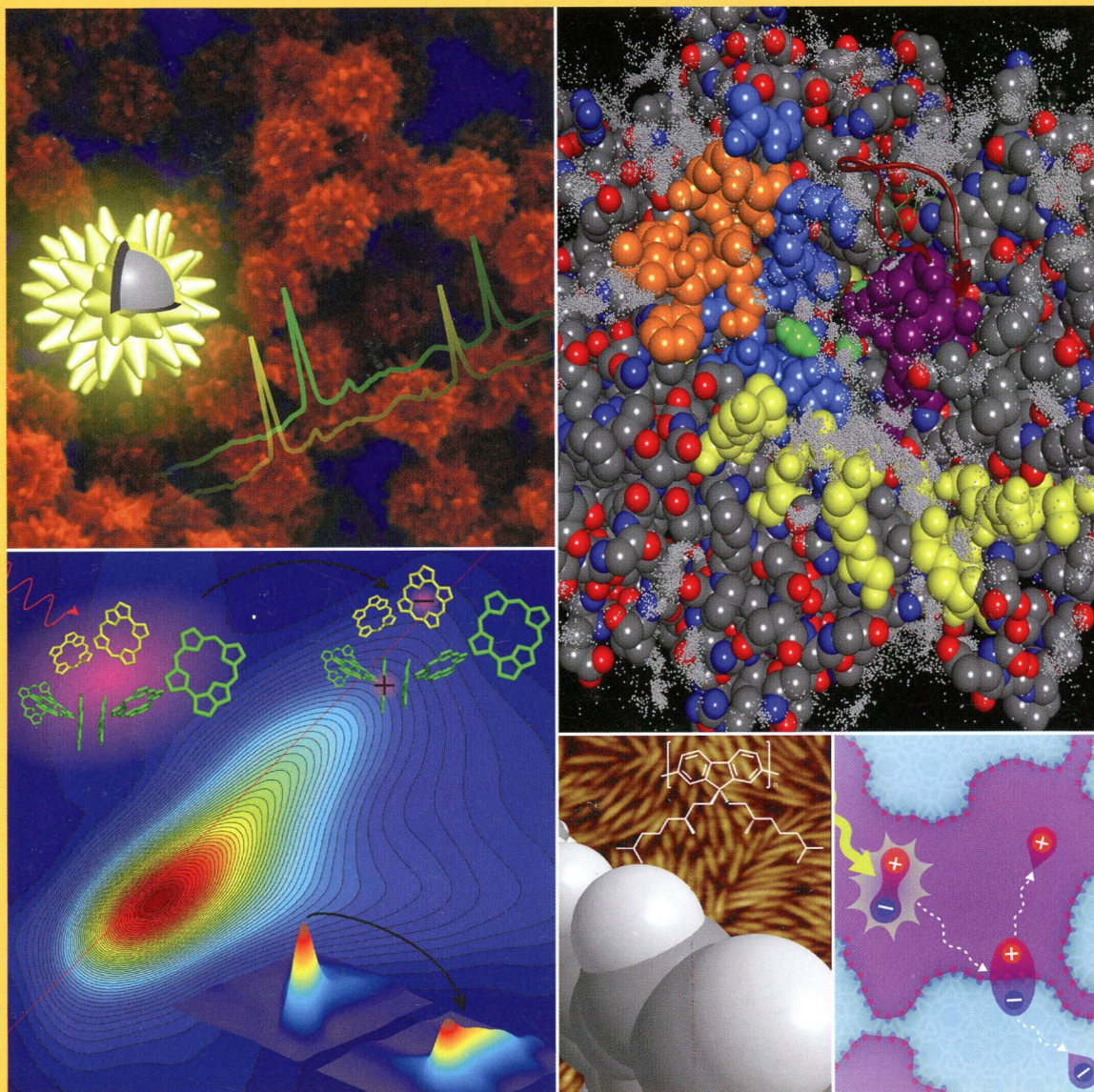
VOLUME 117

NUMBER 22

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

June 6, 2013
Volume 117, Issue 22
Pages 6585-6858

Biophysical Chemistry and Biomolecules

Spectroscopic Study of the Light-Harvesting CP29 Antenna Complex of Photosystem II—Part I

Ximao Feng, Xiaowei Pan, Mei Li, Jörg Pieper, Wenrui Chang, and Ryszard Jankowiak
pp 6585–6592

Publication Date (Web): April 30, 2013 (Article)

DOI: 10.1021/jp4004328

 Section:

Plant Biochemistry

Modeling of Optical Spectra of the Light-Harvesting CP29 Antenna Complex of Photosystem II—Part II

Ximao Feng, Adam Kell, Jörg Pieper, and Ryszard Jankowiak
pp 6593–6602

Publication Date (Web): May 12, 2013 (Article)

DOI: 10.1021/jp4004278

 Section:

Plant Biochemistry

Binding Mechanism of Inositol Stereoisomers to Monomers and Aggregates of A β (16-22)

Grace Li and Régis Pomès
pp 6603–6613

Publication Date (Web): April 29, 2013 (Article)

DOI: 10.1021/jp311350r

 Section:

Pharmacology

Effect of Ionic Aqueous Environments on the Structure and Dynamics of the A β _{21–30} Fragment: A Molecular-Dynamics Study

Micholas Dean Smith and Luis Cruz
pp 6614–6624

Publication Date (Web): May 15, 2013 (Article)

DOI: 10.1021/jp312653h

Section:

General Biochemistry

NMR Relaxation in Proteins with Fast Internal Motions and Slow Conformational Exchange: Model-Free Framework and Markov State Simulations

Junchao Xia, Nan-jie Deng, and Ronald M. Levy

pp 6625–6634

Publication Date (Web): May 2, 2013 (Article)

DOI: 10.1021/jp400797y

Section:

Enzymes

Catalytic Mechanism of Angiotensin-Converting Enzyme and Effects of the Chloride Ion

Chunchun Zhang, Shanshan Wu, and Dingguo Xu

pp 6635–6645

Publication Date (Web): May 15, 2013 (Article)

DOI: 10.1021/jp400974n

Section:

Enzymes

Overdamped Dynamics of Folded Protein Domains within a Locally Harmonic Basin Using Coarse Graining Based on a Partition of Compact Flexible Clusters

Anthony C. Manson and Rob D. Coalson

pp 6646–6655

Publication Date (Web): May 3, 2013 (Article)

DOI: 10.1021/jp4017147

Section:

General Biochemistry

Nonempirical Energetic Analysis of Reactivity and Covalent Inhibition of Fatty Acid Amide Hydrolase

Ewa I. Chudyk, Edyta Dyguda-Kazimierowicz, Karol M. Langner, W. Andrzej Sokalski, Alessio Lodola, Marco Mor, Jitnapa Sirirak, and Adrian J. Mulholland

pp 6656–6666

Publication Date (Web): May 8, 2013 (Article)

DOI: 10.1021/jp401834v

Section:

Enzymes

Molecular Dynamics Simulations of Membrane–Sugar Interactions

Jon Kapla, Jakob Wohler, Baltzar Stevansson, Olof Engström, Göran Widmalm, and Arnold Maliniak

pp 6667–6673

Publication Date (Web): May 10, 2013 (Article)

DOI: 10.1021/jp402385d



ACS Section:

General Biochemistry

Insights on the Binding of Thioflavin Derivative Markers to Amyloid-Like Fibril Models from Quantum Chemical Calculations

Jorge Alí-Torres, Albert Rimola, Cristina Rodríguez-Rodríguez, Luis Rodríguez-Santiago, and Mariona Sodupe

pp 6674–6680

Publication Date (Web): May 10, 2013 (Article)

DOI: 10.1021/jp402807g

ACS Section:

General Biochemistry

Sum-Frequency-Generation Vibration Spectroscopy and Density Functional Theory Calculations with Dispersion Corrections (DFT-D2) for Cellulose I α and I β

Christopher M. Lee, Naseer M. A. Mohamed, Heath D. Watts, James D. Kubicki, and Seong H. Kim

pp 6681–6692

Publication Date (Web): May 29, 2013 (Article)

DOI: 10.1021/jp402998s

ACS Section:

Physical Organic Chemistry

2D $^1\text{H}/^1\text{H}$ RFDR and NOESY NMR Experiments on a Membrane-Bound Antimicrobial Peptide Under Magic Angle Spinning

Ayyalusamy Ramamoorthy and Jiadi Xu

pp 6693–6700

Publication Date (Web): May 14, 2013 (Article)

DOI: 10.1021/jp4034003

ACS Section:

Biochemical Methods

Insights into the Catalytic Mechanism of Coral Allene Oxide Synthase: A Dispersion Corrected Density Functional Theory Study

Eric A. C. Bushnell, Rami Gherib, and James W. Gauld

pp 6701–6710

Publication Date (Web): May 15, 2013 (Article)

DOI: 10.1021/jp403405b

 Section:

Enzymes

Interaction of G-Quadruplex with RecA Protein Studied in Bulk Phase and at the Single-Molecule Level

Atsushi Tanaka, Jungkweon Choi, Seog K. Kim, and Tetsuro Majima

pp 6711–6717

Publication Date (Web): May 10, 2013 (Article)

DOI: 10.1021/jp4036277

 Section:

General Biochemistry

Analysis of Biomolecular Solvation Sites by 3D-RISM Theory

Daniel J. Sindhikara and Fumio Hirata

pp 6718–6723

Publication Date (Web): May 15, 2013 (Article)

DOI: 10.1021/jp4046116

 Section:

Biochemical Methods

Biomaterials, Surfactants, and Membranes

Interfacial Phenomena during Salt Layer Formation under High Rate Dissolution Conditions

Joshua A. Hammons, Alison J. Davenport, S. Majid Ghahari, Mehdi Monir, Jean-Phillipe Tinnes, Mahrez Amri, Nick Terrill, Federica Marone, Rajmund Mokso, Marco Stampanoni, and Trevor Rayment

pp 6724–6732

Publication Date (Web): April 18, 2013 (Article)

DOI: 10.1021/jp311666w

 Section:

Electrochemistry

Self-Assembly of Patterned Nanoparticles on Cellular Membranes: Effect of Charge Distribution

Ye Li, Xianren Zhang, and Dapeng Cao

pp 6733–6740

Publication Date (Web): May 13, 2013 (Article)

DOI: 10.1021/jp312124x

 Section:

Pharmaceuticals

Phospholipid–Lactose Permease Interaction As Reported by a Head-Labeled Pyrene Phosphatidylethanolamine: A FRET Study

Carme Suárez-Germà, Luís M. S. Loura, Manuel Prieto, Òscar Domènech, Josep M. Campanera, M. Teresa Montero, and Jordi Hernández-Borrell

pp 6741–6748

Publication Date (Web): May 6, 2013 (Article)

DOI: 10.1021/jp402152n

 Section:

General Biochemistry

Single-Walled Carbon Nanotubes Do Not Pierce Aqueous Phospholipid Bilayers at Low Salt Concentration

Liu Shi, Dachuan Shi, Matthias U. Nollert, Daniel E. Resasco, and Alberto Striolo

pp 6749–6758

Publication Date (Web): May 9, 2013 (Article)

DOI: 10.1021/jp4039336

 Section:

General Biochemistry

Liquids; Chemical and Dynamical Processes in Solution

Ab Initio Study on an Excited-State Intramolecular Proton-Transfer Reaction in Ionic Liquid

Seigo Hayaki, Yoshifumi Kimura, and Hirofumi Sato

pp 6759–6767

Publication Date (Web): May 22, 2013 (Article)

DOI: 10.1021/jp311883f

 Section:

General Physical Chemistry

Prediction of Fundamental Properties of Ionic Liquid Electrospray Thrusters using Molecular Dynamics

Arnaud Borner, Zheng Li, and Deborah A. Levin

pp 6768–6781

Publication Date (Web): May 9, 2013 (Article)

DOI: 10.1021/jp402092e

 Section:

Propellants and Explosives

Hydrogen Production in Aromatic and Aliphatic Ionic Liquids

Surajdevprakash B. Dhiman, George S. Goff, Wolfgang Runde, and Jay A. LaVerne

pp 6782–6788

Publication Date (Web): May 15, 2013 (Article)

DOI: 10.1021/jp402502d

 Section:

Physical Organic Chemistry

Roles of Viscosity, Polarity, and Hydrogen-Bonding Ability of a Pyrrolidinium Ionic Liquid and Its Binary Mixtures in the Photophysics and Rotational Dynamics of the Potent Excited-State Intramolecular Proton-Transfer Probe 2,2'-Bipyridine-3,3'-diol

Sarthak Mandal, Surajit Ghosh, Chiranjib Banerjee, Jagannath Kuchlyan, and Nilmoni Sarkar

pp 6789–6800

Publication Date (Web): May 13, 2013 (Article)

DOI: 10.1021/jp4025443

 Section:

Physical Organic Chemistry

Glasses, Colloids, Polymers, and Soft Matter

Computationally Efficient Methodology for Atomic-Level Characterization of Dendrimer–Drug Complexes: A Comparison of Amine- and Acetyl-Terminated PAMAM

Ariela Vergara-Jaque, Jeffrey Comer, Luis Monsalve, Fernando D. González-Nilo, and Claudia Sandoval

pp 6801–6813

Publication Date (Web): May 3, 2013 (Article)

DOI: 10.1021/jp4000363

 Section:

Pharmaceuticals

Ions-Induced Nanostructuring: Effect of Specific Ionic Adsorption on Hydrophobic Polymer Surfaces

Igor Siretanu, Jean-Paul Chapel, Delfi Bastos-González, and Carlos Drummond
pp 6814–6822

Publication Date (Web): May 7, 2013 (Article)

DOI: 10.1021/jp400531x

 Section:

Surface Chemistry and Colloids

The Local Structure and Vibrational Properties of BaTi₂O₅ Glass Revealed by Molecular Dynamics Simulation

Hiroyuki Inoue, Atsunobu Masuno, Shinji Kohara, and Yasuhiro Watanabe
pp 6823–6829

Publication Date (Web): May 6, 2013 (Article)

DOI: 10.1021/jp401730f

 Section:

Crystallography and Liquid Crystals

Structural Analysis of a Banana-Liquid Crystal in the B₄ Phase by Solid-State NMR

Kazuhiko Yamada, Sungmin Kang, Koji Takimoto, Masaya Hattori, Kei Shirata, Susumu Kawauchi, Kenzo Deguchi, Tadashi Shimizu, and Junji Watanabe
pp 6830–6838

Publication Date (Web): May 8, 2013 (Article)

DOI: 10.1021/jp402237y

 Section:

Physical Organic Chemistry

Layer-by-Layer Film Growth Using Polysaccharides and Recombinant Polypeptides: A Combinatorial Approach

Rui R. Costa, Ana M. Testera, F. Javier Arias, J. Carlos Rodríguez-Cabello, and João F. Mano
pp 6839–6848

Publication Date (Web): May 10, 2013 (Article)

DOI: 10.1021/jp4028518

 Section:

Pharmaceuticals

Origin of Attraction in Chalcogen–Nitrogen Interaction of 1,2,5-Chalcogenadiazole Dimers

Seiji Tsuzuki and Naoki Sato
pp 6849–6855

Publication Date (Web): May 9, 2013 (Article)

DOI: 10.1021/jp403200j

 Section:

Physical Organic Chemistry

Additions and Corrections

Correction to Accelerated Particle-Based Target Capture— The Roles of Volume Transport and Near-Surface Alignment

Alexander van Reenen, Arthur M. de Jong, and Menno W. J. Prins

pp 6856–6856

Publication Date (Web): May 24, 2013 (Addition/Correction)

DOI: 10.1021/jp403354p

 Section:

Biochemical Methods

Correction to “Multidonor Deep-UV FRET Study of Protein–Ligand Binding and Its Potential to Obtain Structure Information”

Qiang Li, Dorinel Verdes, and Stefan Seeger

pp 6857–6857

Publication Date (Web): May 28, 2013 (Addition/Correction)

DOI: 10.1021/jp403771p

 Section:

Biochemical Methods

Correction to Comparison of Two Simple Models for High Frequency Friction: Exponential versus Gaussian Wings

Steven A. Adelman

pp 6858–6858

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

DOI: 10.1021/jp4043107

 Section:

General Physical Chemistry