

THE JOURNAL OF PHYSICAL CHEMISTRY B



Larger Cover

February 7, 2013

Volume 117, Issue 5

Pages 1197-1500

Biophysical Chemistry and Biomolecules

Theoretical Simulations on Interactions of Mono- and Dinuclear Metallonucleases with DNA

Chunmei Liu, Yanyan Zhu, Peipei Chen, and Mingsheng Tang

pp 1197–1209

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

DOI: 10.1021/jp306998f



Section:

Enzymes

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 1210–1218

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

DOI: 10.1021/jp307862h



Section:

Biochemical Methods

Efficient Transformation of Parahydrogen Spin Order into Heteronuclear Magnetization

Chong Cai, Aaron M. Coffey, Roman V. Shchepin, Eduard Y. Chekmenev, and Kevin W. Waddell

pp 1219–1224

Publication Date (Web): December 7, 2012 (Article)

DOI: 10.1021/jp3089462



Section:

Magnetic Phenomena

Organization and Dynamics of the N-Terminal Domain of Chemokine Receptor CXCR1 in Reverse Micelles: Effect of Graded Hydration

Arunima Chaudhuri, Pritam Basu, Sourav Haldar, Mamata Kombrabail, G. Krishnamoorthy, Krishna Rajarathnam, and Amitabha Chattopadhyay

pp 1225–1233

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

DOI: 10.1021/jp3095352

 Section:

General Biochemistry

Microviscosity-Induced Conformational Transition in β -Lactoglobulin in the Presence of an Ionic Liquid

Kamatchi Sankaranarayanan, B. Sreedhar, B.U. Nair, and A. Dhathathreyan

pp 1234–1240

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

DOI: 10.1021/jp310198f

 Section:

General Biochemistry

Revisiting Point FRAP to Quantitatively Characterize Anomalous Diffusion in Live Cells

Matthew K. Daddysman and Christopher J. Fecko

pp 1241–1251

Publication Date (Web): January 11, 2013 (Article)

DOI: 10.1021/jp310348s

 Section:

Biochemical Methods

Time-Resolved Single Molecule Fluorescence Spectroscopy of an α -Chymotrypsin Catalyzed Reaction

Tatyana G. Terentyeva, Johan Hofkens, Tamiki Komatsuzaki, Kerstin Blank, and Chun-Biu Li

pp 1252–1260

Publication Date (Web): January 11, 2013 (Article)

DOI: 10.1021/jp310663v

 Section:

Enzymes

pH-Responsive Mechanism of a Deoxycholic Acid and Folate Comodified Chitosan Micelle under Cancerous Environment

Daiqin Chen, Peng Song, Feng Jiang, Xiangyue Meng, Weiping Sui, Chunying Shu, and Li-Jun Wan

pp 1261–1268

Publication Date (Web): January 11, 2013 (Article)

DOI: 10.1021/jp310677p

 Section:

Pharmaceuticals

The Role of Amino Acid Sequence in the Self-Association of Therapeutic Monoclonal Antibodies: Insights from Coarse-Grained Modeling

Anuj Chaudhri, Isidro E. Zarraga, Sandeep Yadav, Thomas W. Patapoff, Steven J. Shire, and Gregory A. Voth

pp 1269–1279

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

DOI: 10.1021/jp3108396

 Section:

General Biochemistry

Spatial Orientation and Electric-Field-Driven Transport of Hypericin Inside of Bilayer Lipid Membranes

Alena Strejčková, Jana Staničová, Daniel Jancura, Pavol Miškovský, and Gregor Bánó

pp 1280–1286

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

DOI: 10.1021/jp3114539

 Section:

General Biochemistry

Binding Sites of Resveratrol, Genistein, and Curcumin with Milk α - and β -Caseins

P. Bourassa, J. Bariyanga, and H. A. Tajmir-Riahi

pp 1287–1295

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

DOI: 10.1021/jp3114557

 Section:

Food and Feed Chemistry

Redox Control and Hydrogen Bonding Networks: Proton-Coupled Electron Transfer Reactions and Tyrosine Z in the Photosynthetic Oxygen-Evolving Complex

James M. Keough, Ashley N. Zuniga, David L. Jenson, and Bridgette A. Barry

pp 1296–1307

Publication Date (Web): January 24, 2013 (Article)

DOI: 10.1021/jp3118314

 Section:

Plant Biochemistry

Carbon Relaxation in $^{13}\text{C}^\alpha\text{-H}^\alpha$ and $^{13}\text{C}^\alpha\text{-D}^\alpha$ Spin Pairs as a Probe of Backbone Dynamics in Proteins

Hechao Sun, Dong Long, Rafael Brüschweiler, and Vitali Tugarinov

pp 1308–1320

Publication Date (Web): January 11, 2013 (Article)

DOI: 10.1021/jp312292k

 Section:

Biochemical Methods

Exploring the Active Site Structure of a Photoreceptor Protein by Raman Optical Activity

Masashi Unno, Takashi Kikukawa, Masato Kumauchi, and Naoki Kamo

pp 1321–1325

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

DOI: 10.1021/jp4001187

 Section:

Biochemical Methods

Determinants of Regioselectivity and Chemoselectivity in Fosfomycin Resistance Protein FosA from QM/MM Calculations

Rong-Zhen Liao and Walter Thiel

pp 1326–1336

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

DOI: 10.1021/jp4002719

 Section:

Enzymes

Biomaterials, Surfactants, and Membranes

Interparticle Dispersion, Membrane Curvature, and Penetration Induced by Single-Walled Carbon Nanotubes Wrapped with Lipids and PEGylated Lipids

Hwankyu Lee

pp 1337–1344

Publication Date (Web): December 6, 2012 (Article)

DOI: 10.1021/jp308912r

 Section:
Pharmaceuticals

How Do Anions Affect Self-Assembly and Solubility of Cetylpyridinium Surfactants in Water

Wolfram Müller, Christophe Déjugnat, Thomas Zemb, Jean-François Dufrêche, and Olivier Diat
pp 1345–1356

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

DOI: 10.1021/jp3093622

 Section:

Surface Chemistry and Colloids

Effect of Carbon Spacer Length on Zwitterionic Carboxybetaines

Qing Shao and Shaoyi Jiang

pp 1357–1366

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

DOI: 10.1021/jp3094534

 Section:

Physical Organic Chemistry

Probing the Distribution of Water Molecules Hydrating Lipid Membranes with Ultrafast Förster Vibrational Energy Transfer

L. Piatkowski, J. de Heij, and Huib J. Bakker

pp 1367–1377

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

DOI: 10.1021/jp310602v

 Section:

Biochemical Methods

Liquids; Chemical and Dynamical Processes in Solution

Effects of Water Concentration on the Structural and Diffusion Properties of Imidazolium-Based Ionic Liquid–Water Mixtures

Amir A. Niazi, Brooks D. Rabideau, and Ahmed E. Ismail

pp 1378–1388

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

DOI: 10.1021/jp3080496

 Section:

Phase Equilibria, Chemical Equilibria, and Solutions

A Comparative Study on the Thermophysical Properties for Two Bis[(trifluoromethyl)sulfonyl]imide-Based Ionic Liquids Containing the Trimethyl-Sulfonium or the Trimethyl-Ammonium Cation in Molecular Solvents

Erwan Couadou, Johan Jacquemin, Hervé Galiano, Christopher Hardacre, and Mérièm Anouti
pp 1389–1402

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

DOI: 10.1021/jp308139r

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

Nucleation of Gas Hydrates within Constant Energy Systems

Shuai Liang and Peter G. Kusalik

pp 1403–1410

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

DOI: 10.1021/jp308395x

 Section:

Surface Chemistry and Colloids

Electrical Conductivity of Seven Binary Systems Containing 1-Ethyl-3-methyl Imidazolium Alkyl Sulfate Ionic Liquids with Water or Ethanol at Four Temperatures

E. Rilo, J. Vila, S. García-Garabal, L. M. Varela, and O. Cabeza

pp 1411–1418

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

DOI: 10.1021/jp309891j

 Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

Water Evaporation: A Transition Path Sampling Study

Patrick Varilly and David Chandler

pp 1419–1428

Publication Date (Web): December 14, 2012 (Article)

DOI: 10.1021/jp310070y

 Section:

General Physical Chemistry

Relaxation and Dissociation Following Photoexcitation of the $(\mu\text{-N}_2)[\text{Mo}(\text{N}[\text{t-Bu}]\text{Ar})_3]_2$ Dinitrogen Cleavage Intermediate

Adam S. Huss, John J. Curley, Christopher C. Cummins, and David A. Blank

pp 1429–1436

Publication Date (Web): December 18, 2012 (Article)

DOI: 10.1021/jp310122x

 Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Glasses, Colloids, Polymers, and Soft Matter

Mechanism of Solid State Amorphization of Glucose upon Milling

N. Dujardin, J. F. Willart, E. Dudognon, F. Danède, and M. Descamps

pp 1437–1443

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

DOI: 10.1021/jp3069267

 Section:

Physical Organic Chemistry

Mid-Range Structure of Niobium–Sodium–Phosphate Electro-Optic Glasses

A. A. Lipovskii, D. K. Tagantsev, I. E. Apakova, T. S. Markova, O. V. Yanush, M.G. Donato, L. Sirleto, G. Messina, and G. C. Righini

pp 1444–1450

Publication Date (Web): December 31, 2012 (Article)

DOI: 10.1021/jp3081244

 Section:

Ceramics

Temperature-Induced Reversible Transition between Vesicle and Supramolecular Hydrogel in the Aqueous Ionic Liquid– β -Cyclodextrin System

Jingjing Zhang and Xinghai Shen

pp 1451–1457

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

DOI: 10.1021/jp308877w

 Section:

Surface Chemistry and Colloids

Nondestructive Characterization of Li⁺ Ion-Doped Multifunctional Poly(vinylidene fluoride)-g-poly(dimethyl amino ethyl methacrylate) by Impedance Spectroscopy

Pratap Mukherjee, Aniruddha Kundu, Sanjoy Samanta, Somnath Roy, and Arun K. Nandi

pp 1458–1466

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

DOI: 10.1021/jp311755w

 Section:

Physical Properties of Synthetic High Polymers

Improved Self-Healing of Polyethylene/Carbon Black Nanocomposites by Their Shape Memory Effect

Xiaoyan Wang, Jun Zhao, Min Chen, Lan Ma, Xiaodong Zhao, Zhi-Min Dang, and Zhenwen Wang

pp 1467–1474

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

DOI: 10.1021/jp3098796

 Section:

Plastics Manufacture and Processing

Rheological Study of Mutarotation of Fructose in Anhydrous State

Yangyang Wang, Patryk Wlodarczyk, Alexei P. Sokolov, and Marian Paluch

pp 1475–1479

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

DOI: 10.1021/jp310471b

 Section:

Carbohydrates

Phase Boundaries, Structural Characteristics, and NMR Spectra of Ionic Liquid-in-Oil Microemulsions Containing Double Chain Surface Active Ionic Liquid: A Comparative Study

Vishal Govind Rao, Sarthak Mandal, Surajit Ghosh, Chiranjib Banerjee, and Nilmoni Sarkar

pp 1480–1493

Publication Date (Web): January 11, 2013 (Article)

DOI: 10.1021/jp310616p

 Section:

Surface Chemistry and Colloids

Crystallization and Dissolution Behavior of Naproxen/Polyethylene Glycol Solid Dispersions

Qing Zhu, Scott J. Toth, Garth J. Simpson, Hsin-Yun Hsu, Lynne S. Taylor, and Michael T. Harris

pp 1494–1500

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

DOI: 10.1021/jp3106716