# THE JOURNAL OF PHYSICAL CHEMISTRY B

July 3, 2013

Volume 117, Issue 26

Pages 7849-8046

#### Biophysical Chemistry and Biomolecules

Car-Parrinello Molecular Dynamics/Molecular Mechanics (CPMD/MM) Simulation Study of Coupling and Uncoupling Mechanisms of Cytochrome P450cam

Peng Lian, Jue Li, Dong-Qi Wang, and Dong-Qing Wei

pp 7849-7856

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

**DOI:** 10.1021/jp312107r

Section:

Enzymes

# Effective and Reversible DNA Condensation Induced by a Simple Cyclic/Rigid Polyamine Containing Carbonyl Moiety

Chao Li, Chunying Ma, Pengxiang Xu, Yuxing Gao, Jin Zhang, Renzhong Qiao, and Yufen Zhao

pp 7857-7867

Publication Date (Web): June 4, 2013 (Article)

**DOI:** 10.1021/jp312766u

Section:

General Biochemistry

#### Sub-millisecond Chain Collapse of the Escherichia coli Globin ApoHmpH

Li Zhu, Neşe Kurt, Jennifer Choi, Lisa J. Lapidus, and Silvia Cavagnero

pp 7868-7877

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

**DOI:** 10.1021/jp400174e

Section:

**General Biochemistry** 

#### Quantitative Local Photosynthetic Flux Measurements at Isolated Chloroplasts and Thylakoid Membranes Using Scanning Electrochemical Microscopy (SECM)

Kim McKelvey, Sophie Martin, Colin Robinson, and Patrick R. Unwin

pp 7878-7888

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

DOI: 10.1021/jp403048f

Section:

**Biochemical Methods** 

#### In Situ Spectroscopic Quantification of Protein-Ice Interactions

Alan Twomey, Rebekah Less, Kosaku Kurata, Hiroshi Takamatsu, and Alptekin Aksan

pp 7889-7897

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

**DOI:** 10.1021/jp403267x

Section:

**Biochemical Methods** 

### Are Time-Dependent Fluorescence Shifts at the Tunnel Mouth of Haloalkane Dehalogenase Enzymes Dependent on the Choice of the Chromophore?

Mariana Amaro, Jan Brezovský, Silvia Kováčová, Lukáš Maier, Radka Chaloupková, Jan Sýkora, Kamil Paruch, Jiří Damborský, and Martin Hof

pp 7898-7906

Publication Date (Web): June 5, 2013 (Article)

DOI: 10.1021/jp403708c

Section:

**Enzymes** 

#### Molecular Details of the Activation of the μ Opioid Receptor

Jihyun Shim, Andrew Coop, and Alexander D. MacKerell, Jr.

pp 7907-7917

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

**DOI:** 10.1021/jp404238n

Section:

**General Biochemistry** 

#### Local Frustration Determines Molecular and Macroscopic Helix Structures

Christopher J. Forman, Szilard N. Fejer, Dwaipayan Chakrabarti, Paul D. Barker, and David J. Wales

pp 7918-7928

Publication Date (Web): May 31, 2013 (Article)

**DOI:** 10.1021/jp4040503

Section:

**General Biochemistry** 

#### Biomaterials, Surfactants, and Membranes Edelfosine and Miltefosine Effects on Lipid Raft Properties: Membrane Biophysics in Cell Death by Antitumor Lipids

Bruno M. Castro, Aleksander Fedorov, Valentin Hornillos, Javier Delgado, A Ulises Acuña, Faustino Mollinedo, and Manuel Prieto

pp 7929-7940

Publication Date (Web): June 5, 2013 (Article)

**DOI:** 10.1021/jp401407d

Section:

**General Biochemistry** 

# Proton Transport Pathways in an Acid-Base Complex Consisting of a Phosphonic Acid Group and a 1,2,3-Triazolyl Group

Baohua Yue, Liuming Yan, Shuaiyuan Han, and Liqing Xie

pp 7941-7949

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

**DOI:** 10.1021/jp404684e

Section:

**Physical Organic Chemistry** 

### Adsorption of Sodium Dodecyl Sulfate on Functionalized Graphene Measured by Conductometric Titration

Andrew G. Hsieh, Christian Punckt, Sibel Korkut, and Ilhan A. Aksay

pp 7950-7958

Publication Date (Web): June 4, 2013 (Article)

**DOI:** 10.1021/jp403876t

Section:

Surface Chemistry and Colloids

#### Ganglioside Influence on Phospholipid Films Investigated with Single Molecule Fluorescence Measurements

Kevin P. Armendariz and Robert C. Dunn

pp 7959-7966

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

**DOI:** 10.1021/jp405312a

Section:

**Biochemical Methods** 

Liquids; Chemical and Dynamical Processes in Solution Anisotropic Dielectric Relaxation of the Water Confined in Nanotubes for Terahertz Spectroscopy Studied by Molecular Dynamics Simulations

Wenpeng Qi, Jige Chen, Junwei Yang, Xiaoling Lei, Bo Song, and Haiping Fang

pp 7967-7971

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

**DOI:** 10.1021/jp3120435

Section:

Electric Phenomena

## Cation Effects on Rotational Dynamics of Anions and Water Molecules in Alkali (Li+, Na+, K+, Cs+) Thiocyanate (SCN-) Aqueous Solutions

Hongtao Bian, Hailong Chen, Qiang Zhang, Jiebo Li, Xiewen Wen, Wei Zhuang, and Junrong Zheng

pp 7972-7984

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

**DOI:** 10.1021/jp4016646

Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

## Intermolecular/Interionic Vibrations of 1-Methyl-3-n-octylimidazolium Tetrafluoroborate Ionic Liquid and Benzene Mixtures

Hideaki Shirota

pp 7985-7995

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

**DOI:** 10.1021/jp402456g

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

# Efficient Parallel Implementations of QM/MM-REMD (Quantum Mechanical/Molecular Mechanics-Replica-Exchange MD) and Umbrella Sampling: Isomerization of $H_2O_2$ in Aqueous Solution

Dmitri G. Fedorov, Yuji Sugita, and Cheol Ho Choi

pp 7996-8002

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

DOI: 10.1021/jp4029529

Section:

**General Physical Chemistry** 

#### Ionic Conductivity and Glass Transition of Phosphoric Acids

Yangyang Wang, Nathan A. Lane, Che-Nan Sun, Fei Fan, Thomas A. Zawodzinski, and Alexei P. Sokolov

pp 8003-8009

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

DOI: 10.1021/jp403867a

Section:

**General Physical Chemistry** 

## Computational Investigation of the Hydration of Alkyl Diammonium Chlorides and Their Effect on THF/Water Phase Separation

Soran Jahangiri, Sean M. Mercer, Philip G. Jessop, and Gilles H. Peslherbe

pp 8010-8017

Publication Date (Web): June 4, 2013 (Article)

DOI: 10.1021/jp403984q

Section:

Phase Equilibriums, Chemical Equilibriums, and Solutions

### Using Monte Carlo Simulation to Compute Liquid-Vapor Saturation Properties of Ionic Liquids

Kaustubh S. Rane and Jeffrey R. Errington

pp 8018-8030

Publication Date (Web): June 5, 2013 (Article)

**DOI:** 10.1021/jp404207x

Section:

**General Physical Chemistry** 

#### Glasses, Colloids, Polymers, and Soft Matter Swarming Behavior of Gradient-Responsive Colloids with Chemical Signaling

Peter Grančič and František Štěpánek

pp 8031-8038

Publication Date (Web): June 4, 2013 (Article)

**DOI:** 10.1021/jp400234n

Section:

**Surface Chemistry and Colloids** 

# Organogels from Dimeric Bile Acid Esters: In Situ Formation of Gold Nanoparticles

Arkajyoti Chakrabarty and Uday Maitra

pp 8039-8046

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

**DOI:** 10.1021/jp4029497

Section:

**Surface Chemistry and Colloids**