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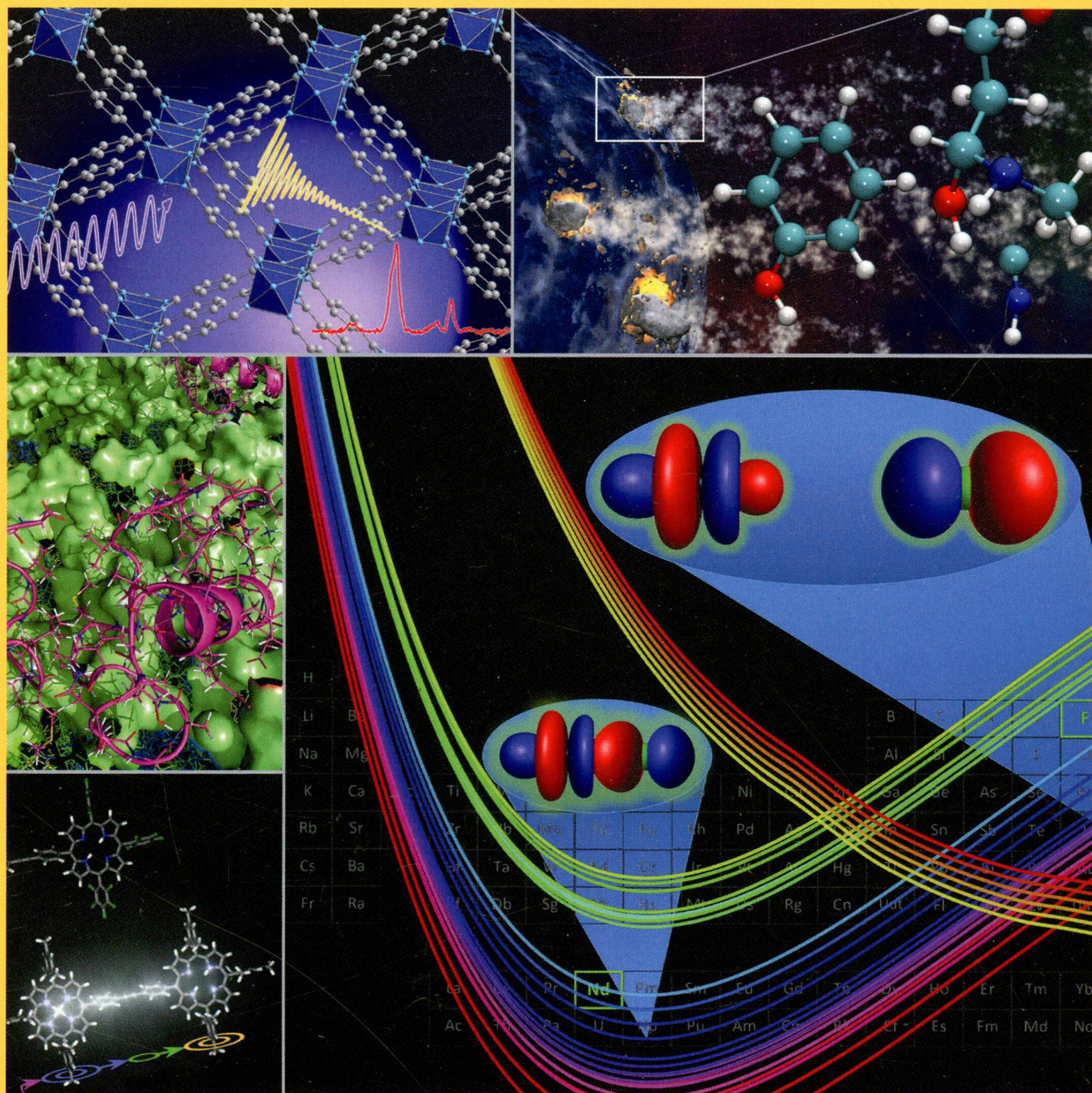
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ON THE COVER: Collage of cover art from recent issues of *J. Phys. Chem.* Top Left: ^{17}O Solid-State NMR Spectra Provide Signatures of Various Oxygen Species in Metal-Organic Frameworks (*J. Phys. Chem. C* **2013**, *117* (33), 16953–16960). Center Left: Behavior of Amyloid β -Peptides on a Ganglioside-Containing Membrane Surface (*J. Phys. Chem. B* **2013**, *117* (27), 8085–8094). Bottom Left: Bridge-Mediated EET in Porphyrin Dimers: Electronic Coupling Reduced by Fluorination (*J. Phys. Chem. C* **2013**, *117* (24), 12423–12431). Top Right: Synthesis of Prebiotic Hydrocarbons in Impacts of Simple Icy Mixtures on Early Earth (*J. Phys. Chem. A* **2013**, *117* (24), 5124–5131). Bottom Right: Computed Potential Energy Curves for Quartet, Doublet, and Sextet States of NdF^{2+} (*J. Phys. Chem. A* **2013**, *117* (42), 10881–10888).

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Biophysical Chemistry and Biomolecules

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DOI: 10.1021/jp5059287

Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model

Wiktoria Giedroyć-Piasecka, Edyta Dyguda-Kazimierowicz,* Wiktor Beker, Marco Mor, Alessio Lodola, and W. Andrzej Sokalski

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DOI: 10.1021/jp506579a

Microsecond Molecular Dynamics Simulations Provide Insight into the Allosteric Mechanism of the Gs Protein Uncoupling from the β_2 Adrenergic Receptor

Xianqiang Sun, Hans Ågren, and Yaoquan Tu*

14745



DOI: 10.1021/jp5075913

Comparison of Optimal Thermodynamic Models of the Tricarboxylic Acid Cycle from Heterotrophs, Cyanobacteria, and Green Sulfur Bacteria

Dennis G. Thomas, Sebastian Jaramillo-Riveri, Douglas J. Baxter, and William R. Cannon*

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Signaling-State Formation Mechanism of a BLUF Protein PapB from the Purple Bacterium *Rhodospseudomonas palustris* Studied by Femtosecond Time-Resolved Absorption Spectroscopy

Tomotsumi Fujisawa, Satoshi Takeuchi, Shinji Masuda, and Tahei Tahara*

14774



DOI: 10.1021/jp508019a

Gas-Phase Conformations and Energetics of Protonated 2'-Deoxyguanosine and Guanosine: IRMPD Action Spectroscopy and Theoretical Studies

R. R. Wu, Bo Yang, G. Berden, J. Oomens, and M. T. Rodgers*

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DOI: 10.1021/jp508751s

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DOI: 10.1021/jp5089096

Water Dynamics at Protein–Protein Interfaces: Molecular Dynamics Study of Virus–Host Receptor Complexes

Priyanka Dutta, Mohsen Botlani, and Sameer Varma*

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DOI: 10.1021/jp5093493

Solvent Stability Study with Thermodynamic Analysis and Superior Biocatalytic Activity of *Burkholderia cepacia* Lipase Immobilized on Biocompatible Hybrid Matrix of Poly(vinyl alcohol) and Hypromellose

Kirtikumar C. Badgujar and Bhalchandra M. Bhanage*

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DOI: 10.1021/jp511056t

Molecular Mechanism of Lead-Induced Superoxide Dismutase Inactivation in Zebrafish Livers

Hao Zhang, Yang Liu, Rutao Liu,* Chunguang Liu, and Yadong Chen

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DOI: 10.1021/jp511702w

Poisson–Boltzmann versus Size-Modified Poisson–Boltzmann Electrostatics Applied to Lipid Bilayers

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Biomaterials, Surfactants, and Membranes

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DOI: 10.1021/jp509348a

Prediction of Phospholipid–Water Partition Coefficients of Ionic Organic Chemicals Using the Mechanistic Model COSMOmic

Kai Bittermann,* Simon Spycher,* Satoshi Endo, Larissa Pohler, Uwe Huniar, Kai-Uwe Goss, and Andreas Klamt

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DOI: 10.1021/jp510747y

Transition of Phase Structures in Mixtures of Lysine and Fatty Acids

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Liquids; Chemical and Dynamical Processes in Solution

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DOI: 10.1021/jp5079604

Importance of Molecular Structure on the Thermophoresis of Binary Mixtures

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14870  DOI: 10.1021/jp509583c

Physical Properties and CO₂ Reaction Pathway of 1-Ethyl-3-Methylimidazolium Ionic Liquids with Aprotic Heterocyclic Anions

Samuel Seo, M. Aruni DeSilva, and Joan F. Brennecke*

14880  DOI: 10.1021/jp5100236

Anion-Functionalized Task-Specific Ionic Liquids: Molecular Origin of Change in Viscosity upon CO₂ Capture

Ailin Li, Ziqi Tian, Tianying Yan,* De-en Jiang,* and Sheng Dai

14888  DOI: 10.1021/jp510672z

Ionic Dynamics in [C₄mim]NTf₂ in the Glassy and Liquid States: Results from ¹³C and ¹H NMR Spectroscopy

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14899  DOI: 10.1021/jp511391b

Structure and Dynamics of Ferrocyanide and Ferricyanide Anions in Water and Heavy Water: An Insight by MD Simulations and 2D IR Spectroscopy

Giacomo Prampolini,* Pengyun Yu, Silvia Pizzanelli, Ivo Cacelli, Fan Yang, Juan Zhao, and Jianping Wang

Glasses, Colloids, Polymers, and Soft Matter

14913 DOI: 10.1021/jp506126d

Interplay of Coil–Globule Transition and Surface Adsorption of a Lattice HP Protein Model

Meng-Bo Luo,* Jesse D. Ziebarth, and Yongmei Wang

14922  DOI: 10.1021/jp506814m

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Makoto Yamaguchi,* Takuro Matsunaga, Kazuki Amemiya, Akihiro Ohira, Naoki Hasegawa, Kazuhiko Shinohara, Masaki Ando, and Toshihiko Yoshida

14929  DOI: 10.1021/jp508244u

Nitrate Concentration near the Surface of Frozen Aqueous Solutions

Harley A. Marrocco and Rebecca R. H. Michelsen*

14942 DOI: 10.1021/jp508910m

Critical V₂O₅/TeO₂ Ratio Inducing Abrupt Property Changes in Vanadium Tellurite Glasses

Jonas Kjeldsen, Ana C. M. Rodrigues, Susanne Mossin, and Yuanzheng Yue*

14949  DOI: 10.1021/jp5089564

Three Rate-Constant Kinetic Model for Permanganate Reactions Autocatalyzed by Colloidal Manganese Dioxide: The Oxidation of L-Phenylalanine

Joaquin F. Perez-Benito* and Jordi Ferrando

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DOI: 10.1021/jp509151w

Formation of a "Hollow" Interior in the Fourth-Generation Dendrimer with Attached Oligomeric Terminal Segments

Denis A. Markelov,* Alexey A. Polotsky, and Tatiana M. Birshtein

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DOI: 10.1021/jp509619t

***In Situ* Infrared Spectroscopy of Oligoaniline Intermediates Created under Alkaline Conditions**

Ivana Šeděnková, Jaroslav Stejskal, and Miroslava Trchová*

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DOI: 10.1021/jp510584w

Phase Behavior and Dynamics of the Liquid Crystal 4'-butyl-4-(2-methylbutoxy)azoxybenzene (4B05*)

E. Juszyńska-Gałązka,* M. Gałązka, M. Massalska-Arodz, A. Bąk, K. Chłędowska, and W. Tomczyk

Additions and Corrections

14990

DOI: 10.1021/jp511974t

Correction to "Structure and Stability of Phospholipid Bilayers Hydrated by a Room-Temperature Ionic Liquid/Water Solution: A Neutron Reflectometry Study"

Antonio Benedetto,* Frank Heinrich, Miguel A. Gonzalez, Giovanna Fragneto, Erik Watkins, and Pietro Ballone