

FM
180/pe

DECEMBER 18, 2014

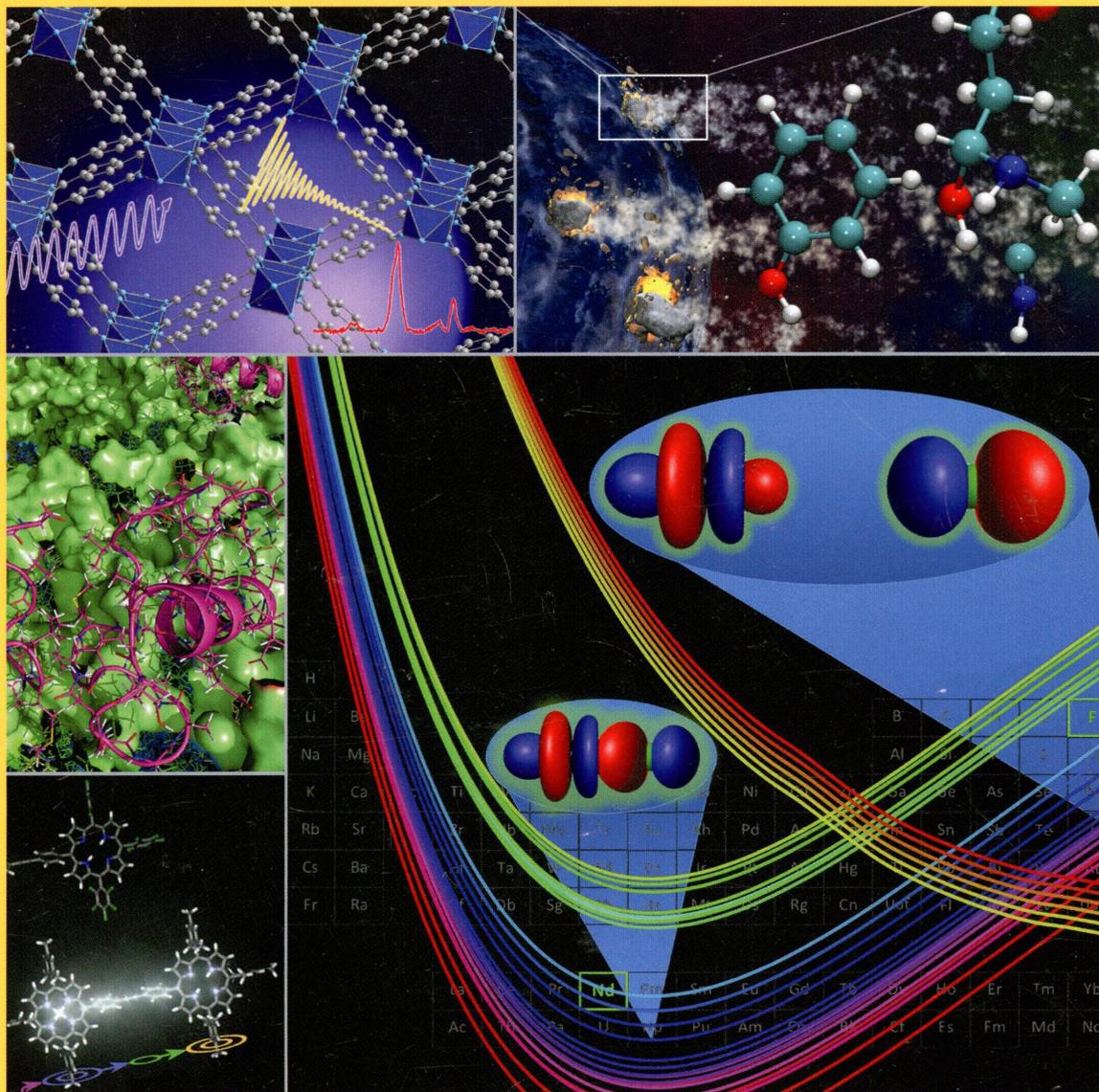
VOLUME 118

NUMBER 50

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

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).

Articles

Biophysical Chemistry and Biomolecules

14555



DOI: 10.1021/jp5065006

Resonance Energy Transfer in DNA Duplexes Labeled with Localized Dyes

Paul D. Cunningham,* Ani Khachatryan, Susan Buckhout-White, Jeffrey R. Deschamps, Ellen R. Goldman, Igor L. Medintz, and Joseph S. Melinger*

14566



DOI: 10.1021/jp507783d

Computational Investigation of Glycosylase and β -Lyase Activity Facilitated by Proline: Applications to FPG and Comparisons to hOgg1

Shahin Sowlati-Hashjin and Stacey D. Wetmore*

14578

DOI: 10.1021/jp509213f

Electric Field as a Disaggregating Agent for Amyloid Fibrils

Andrij Baumketner*

14590



DOI: 10.1021/jp509491p

Relevant Interactions of Antimicrobial Iron Chelators and Membrane Models Revealed by Nuclear Magnetic Resonance and Molecular Dynamics Simulations

João T. S. Coimbra, Tânia Moniz, Natércia F. Brás, Galya Ivanova, Pedro A. Fernandes, Maria J. Ramos,* and Maria Rangel*

14602

DOI: 10.1021/jp5097053

Case Study of Hydrogen Bonding in a Hydrophobic Cavity

Yi-Chen Chen, Chao-Sheng Cheng, Siu-Cin Tjong, Hsien-Sheng Yin,* and Shih-Che Sue*

14612 **S**

DOI: 10.1021/jp510148h

Recommending Hartree–Fock Theory with London-Dispersion and Basis-Set-Superposition Corrections for the Optimization or Quantum Refinement of Protein Structures

Lars Goerigk,* Charles A. Collyer, and Jeffrey R. Reimers*

14627

DOI: 10.1021/jp511126x

Application of Three-Photon Excitation FCS to the Study of Protein Oligomerization

Suman Ranjit, Alexander Dvornikov, David A. Holland, Gregory D. Reinhart, David M. Jameson, and Enrico Gratton*

Biomaterials, Surfactants, and Membranes

14632

DOI: 10.1021/jp5074939

Mechanistic Investigation of Interactions between Steroidal Saponin Digitonin and Cell Membrane Models

Nataliya Frenkel, Ali Makky, Ikhwan Resmala Sudji, Michael Wink,* and Motomu Tanaka*

14640 **S**

DOI: 10.1021/jp507682k

The Relationship between Oxygen Permeability and Phase Separation Morphology of the Multicomponent Silicone Hydrogels

Zhengbai Zhao, Haijiao Xie, Shuangshuang An, and Yong Jiang*

Liquids; Chemical and Dynamical Processes in Solution

14648

DOI: 10.1021/jp510275x

Electrolyte Vortex Dynamics in the Vicinity of a Ferromagnetic Surface in a Direct Current Magnetic Field

Dmytro O. Derecha, Yury B. Skirta, and Igor V. Gerasimchuk*

14652

DOI: 10.1021/jp510420h

Solvatochromic Probe Behavior within Choline Chloride-Based Deep Eutectic Solvents: Effect of Temperature and Water

Ashish Pandey and Siddharth Pandey*

14662 **S**

DOI: 10.1021/jp5104577

Photophysical Investigation of Cyano-Substituted Terrylenediimide Derivatives

Koen Kennes, Yannick Baeten, Tom Vosch, Wouter Sempels, Stoyan Yordanov, Sebastian Stappert, Long Chen, Klaus Müllen, Johan Hofkens, Mark Van der Auweraer, and Eduard Fron*

Glasses, Colloids, Polymers, and Soft Matter

14675

DOI: 10.1021/jp5063786

Role of Precipitating Solute Curvature on Microdrops and Nanodrops during Concentrating Processes: The Nonideal Ostwald–Freundlich Equation

Fatemeh Eslami and Janet A. W. Elliott*

14687

DOI: 10.1021/jp506925x

Breakdown of Time–Temperature Superposition in a Bead–Spring Polymer Melt near the Glass Transition Temperature
Tamio Yamazaki*

14695

DOI: 10.1021/jp508548q

Evaporation Assisted CdSe Nanorod Assembly by Small Angle X-ray Scattering and Langmuir Adsorption
Kimani A. Stancil*

14703

DOI: 10.1021/jp5089355

Dielectric Constant Enhancement of Epoxy Thermosets via Formation of Polyelectrolyte Nanophases
Houluo Cong, Jingang Li, Lei Li, and Sixun Zheng*

14713



DOI: 10.1021/jp510075m

3-Picoline Mediated Self-Assembly of M(II)–Malonate Complexes (M = Ni/Co/Mn/Mg/Zn/Cu) Assisted by Various Weak Forces Involving Lone Pair– π , π – π , and Anion– π –Hole Interactions
Monojit Mitra, Prankrishna Manna, Antonio Bauzá, Pablo Ballester, Saikat Kumar Seth, Somnath Ray Choudhury,*
Antonio Frontera,* and Subrata Mukhopadhyay*

Supporting Information available via online article