

FEBRUARY 13, 2014

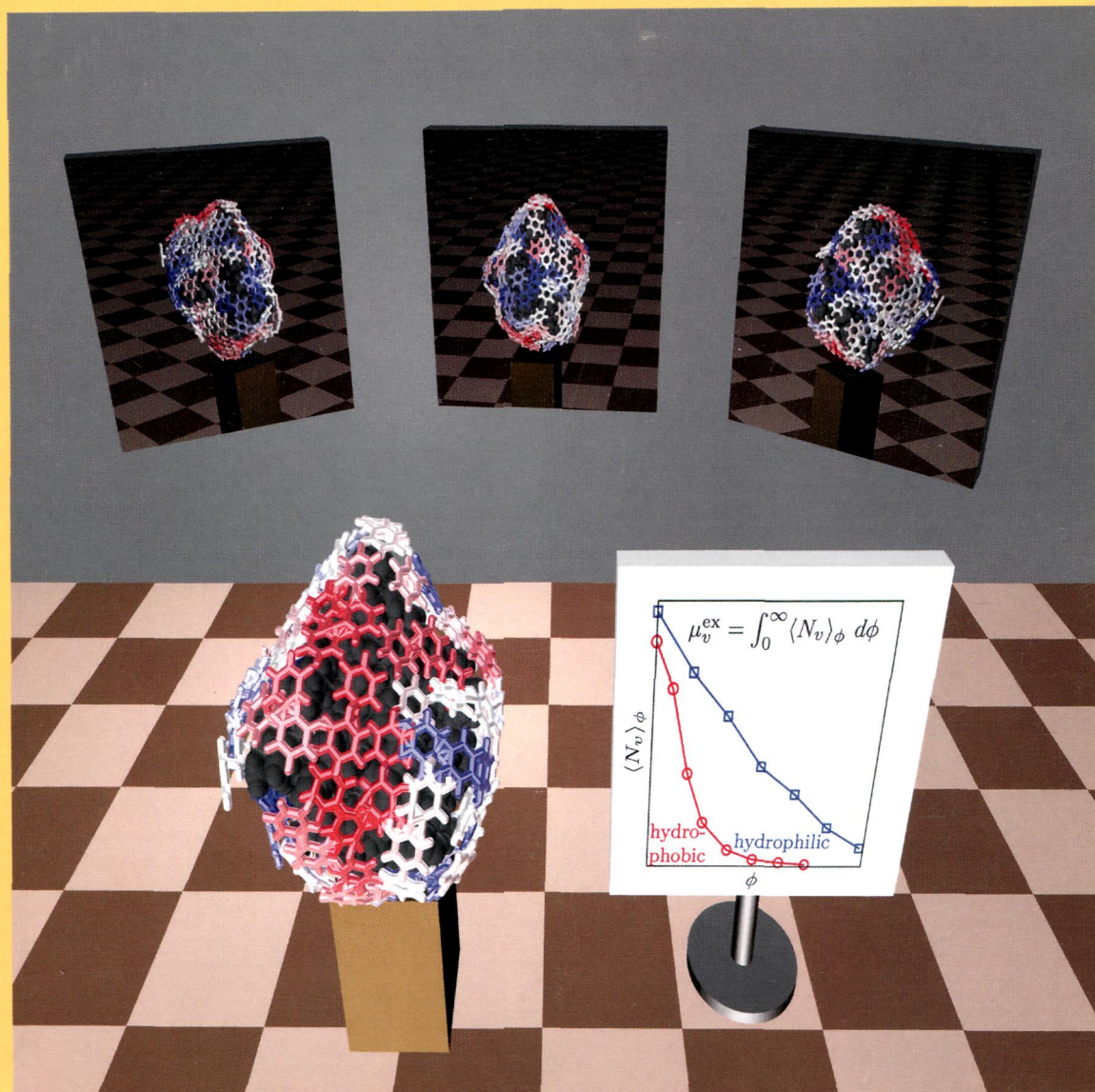
VOLUME 118

NUMBER 6

pubs.acs.org/JPCB

THE JOURNAL OF PHYSICAL CHEMISTRY

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Characterizing the
Hydrophobicity of
Complex Protein
Surfaces Using a
Highly Efficient
Method
(see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: Characterizing the hydrophobicity of complex protein surfaces using a highly efficient, novel method. Accounting for the chemical and topographical complexities of a protein surface in the estimation of its hydrophobicity requires computation of cavity hydration free energies. Using the efficient method (bottom, right), such a context-dependent characterization of hydrophobicity of the protein, hydrophobin II, was carried out using benzene-shaped cavities and is shown here. The reflections of the central protein in the three mirrors placed behind it are also shown. See page 1564.

Review Article


1453 dx.doi.org/10.1021/jp408532r
ZnO Nano Reactor on Textiles and Polymers: Ex Situ and In Situ Synthesis, Application, and Characterization
Majid Montazer and Morteza Maali Amiri*


Articles


Biophysical Chemistry and Biomolecules

1471  dx.doi.org/10.1021/jp408879g
Toward a Molecular Dynamics Force Field for Simulations of 40% Trifluoroethanol–Water
*J. T. Gerig**

1481  dx.doi.org/10.1021/jp4089113
Partitioning of Amino Acids into a Model Membrane: Capturing the Interface
*Taras V. Pogorelov, Josh V. Vermaas, Mark J. Arcario, and Emad Tajkhorshid**

1493  dx.doi.org/10.1021/jp410727r
Large Equatorial Ligand Effects on C–H Bond Activation by Nonheme Iron(IV)-oxo Complexes
*Xiaoli Sun, Caiyun Geng, Ruiping Huo, Ulf Ryde, Yuxiang Bu, and Jilai Li**


1501  dx.doi.org/10.1021/jp411023k
Nuclear Hyperfine and Quadrupole Tensor Characterization of the Nitrogen Hydrogen Bond Donors to the Semiquinone of the Q_B Site in Bacterial Reaction Centers: A Combined X- and S-Band ^{14,15}N ESEEM and DFT Study
Alexander T. Taguchi, Patrick J. O'Malley, Colin A. Wraight,* and Sergei A. Dikanov**

1510  dx.doi.org/10.1021/jp4112662
The Early Steps in the Photocycle of a Photosensor Protein Sensory Rhodopsin I from *Salinibacter ruber*
Yuki Sudo,* Misao Mizuno, Zhengrong Wei, Satoshi Takeuchi, Tahei Tahara,* and Yasuhisa Mizutani*

Biomaterials, Surfactants, and Membranes


1519 dx.doi.org/10.1021/jp406431m
Surface Freezing and Molecular Miscibility of Binary Alkane–Alkane and Fluoroalkane–Alkane Liquid Mixtures
Takanori Takiue,* Mayuko Shimasaki, Miyako Tsuura, Hiroyasu Sakamoto, Hiroki Matsubara, and Makoto Aratono

1527  dx.doi.org/10.1021/jp4106986
Effect of ZnO Nanoparticle and Hexadecyltrimethylammonium Bromide on the Dynamic and Equilibrium Oil–Water Interfacial Tension
Tahereh Fereidooni Moghadam and Saeid Azizian*

1535  dx.doi.org/10.1021/jp410899a
Easily Controlled Grafting of Oligonucleotides on $\gamma\text{Fe}_2\text{O}_3$ Nanoparticles: Physicochemical Characterization of DNA Organization and Biological Activity Studies
Frédéric Geinguenaud, Inès Souissi, Rémi Fagard, Yoann Lalatonne, and Laurence Motte*

1545  dx.doi.org/10.1021/jp412203t
Tracking Single Particles on Supported Lipid Membranes: Multimobility Diffusion and Nanoscopic Confinement
Chia-Lung Hsieh, Susann Spindler, Jens Ehrig, and Vahid Sandoghdar*

Liquids; Chemical and Dynamical Processes in Solution

1555  dx.doi.org/10.1021/jp411782y
Chemical Bonding in Aqueous Ferrocyanide: Experimental and Theoretical X-ray Spectroscopic Study
Nicholas Engel, Sergey I. Bokarev,* Edlira Suljoti, Raul Garcia-Diez, Kathrin M. Lange, Kaan Atak, Ronny Golnak, Alexander Kothe, Marcus Dantz, Oliver Kühn, and Emad F. Aziz*

1564 dx.doi.org/10.1021/jp4081977
Efficient Method To Characterize the Context-Dependent Hydrophobicity of Proteins
Amish J. Patel* and Shekhar Garde*

1574 dx.doi.org/10.1021/jp408603n
Temperature Dependence of Hydrophobic Hydration Dynamics: From Retardation to Acceleration
Elise Duboué-Dijon, Aoife C. Fogarty, and Damien Laage*


1584 dx.doi.org/10.1021/jp4086816
Interaction between SiO_2 and a $\text{KF–KCl–K}_2\text{SiF}_6$ Melt
Yurii P. Zaykov, Andrey V. Isakov,* Irina D. Zakiryanova, Olga G. Reznitskikh, Oleg V. Chemezov, and Alexander A. Redkin

1589  dx.doi.org/10.1021/jp4125765
Polarizable Six-Point Water Models from Computational and Empirical Optimization
Philipp Tröster, Konstantin Lorenzen, and Paul Tavan*


1603 dx.doi.org/10.1021/jp409545x
Automated Optimization of Water–Water Interaction Parameters for a Coarse-Grained Model
Joseph C. Fogarty,* See-Wing Chiu, Peter Kirby, Eric Jakobsson, and Sagar A. Pandit*

1612  dx.doi.org/10.1021/jp411440k
Decomposition of L-Valine under Nonthermal Dielectric Barrier Discharge Plasma
Yingying Li, Arben Kojtari, Gary Friedman, Ari D. Brooks, Alex Fridman, and Hai-Feng Ji*

1621  dx.doi.org/10.1021/jp4115755
The Role of the Cation in the Solvation of Cellulose by Imidazolium-Based Ionic Liquids
Brooks D. Rabideau,* Animesh Agarwal, and Ahmed E. Ismail*

1630  dx.doi.org/10.1021/jp411629m
Probing Electronic Communication for Efficient Light-Harvesting Functionality: Dyads Containing a Common Perylene and a Porphyrin, Chlorin, or Bacteriochlorin
Eunkyung Yang, Jieqi Wang, James R. Diers, Dariusz M. Niedzwiedzki, Christine Kirmaier, David F. Bocian,* Jonathan S. Lindsey,* and Dewey Holten*

Glasses, Colloids, Polymers, and Soft Matter

1648  dx.doi.org/10.1021/jp4092249
Coarse-Graining Poly(ethylene oxide)–Poly(propylene oxide)–Poly(ethylene oxide) (PEO–PPO–PEO) Block Copolymers Using the MARTINI Force Field
Selina Nawaz* and Paola Carbone*

1660 dx.doi.org/10.1021/jp409297t
A Coarse-Grained Model for Epoxy Molding Compound
Shaorui Yang, Zhiwei Cui, and Jianmin Qu*

1670  dx.doi.org/10.1021/jp410589h
Photoresponsive Smectic Liquid Crystalline Multipods and Hyperbranched Azo Polymers
Chinmay G. Nardele and S. K. Asha*

1685  dx.doi.org/10.1021/jp4113188
Construction of Supramolecular Self-Assemblies Based on the Biamphiphilic Ionic Liquid– β -Cyclodextrin System
Jianfeng Shi and Xinghai Shen*

Impact of Dendrimer Surface Functional Groups on the Release of Doxorubicin from Dendrimer Carriers

Mengen Zhang, Rui Guo, Mónika Kéri, István Bányai,* Yun Zheng, Mian Cao, Xueyan Cao, and Xiangyang Shi*