

OCTOBER 9, 2014

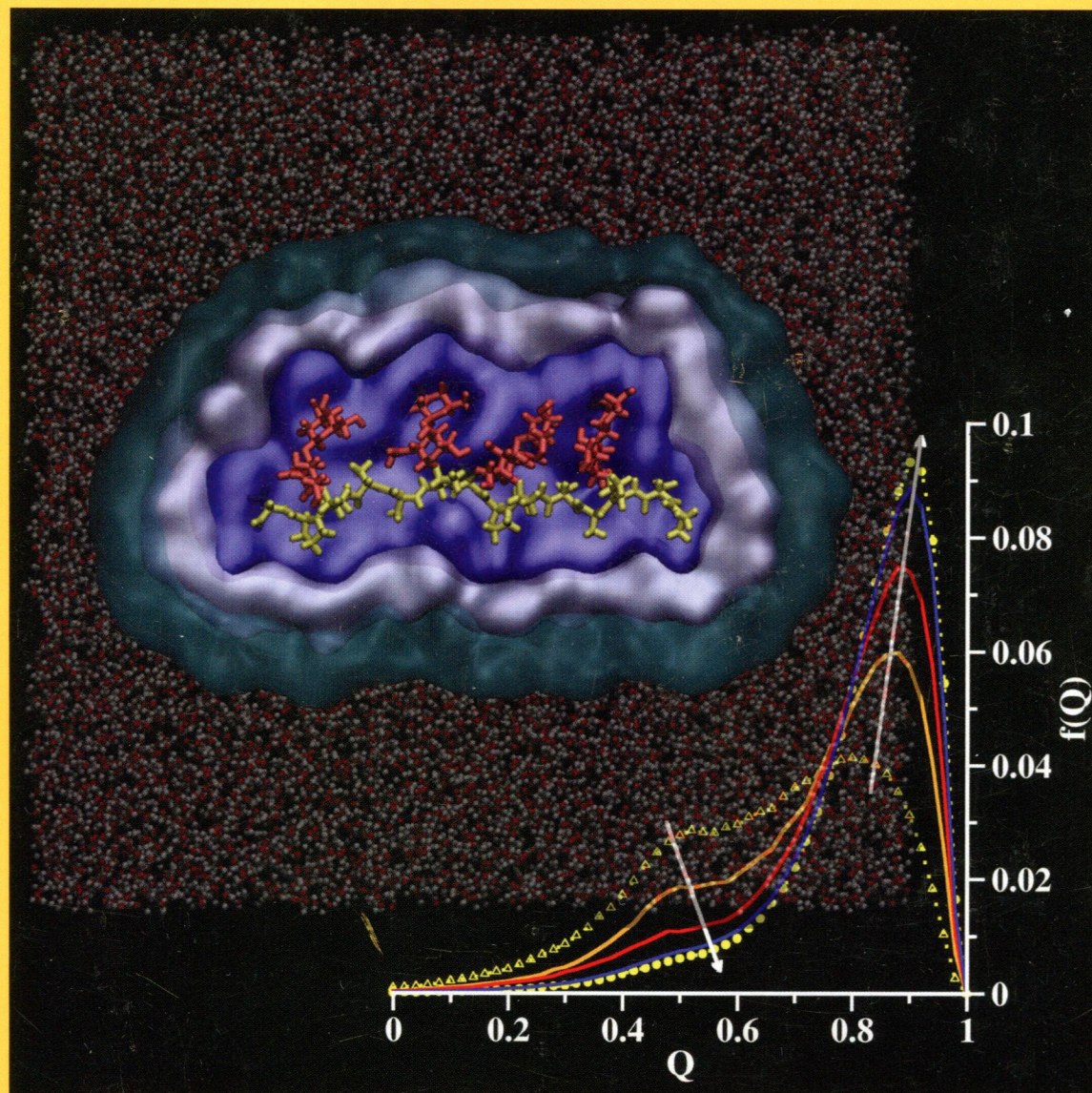
VOLUME 118

NUMBER 40

pubs.acs.org/JPCB

THE JOURNAL OF  
PHYSICAL  
CHEMISTRY

B



Antifreeze Activity  
of the AFGP  
Glycopeptide Involves  
Perturbation of  
Long-Range  
Water Structure  
(see page 11696)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER

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**ON THE COVER:** Antifreeze activity of the AFGP glycopeptide involves perturbation of long-range water structure. Distributions of the local water tetrahedral order parameter,  $Q$ , indicating the disruption of the water structure around the galactose sugars in the AFGP8 glycopeptide at 250 K. Results are shown for water molecules less than 3.5 Å (orange line), between 3.5–5.5 Å (red line), and between 10.0–12.0 Å (blue line) from the galactose sugars.  $Q$  distribution for unperturbed water at 250 K (yellow closed circles) and 300 K (yellow open triangles) are also shown. See page 11696.

## Articles

### Biophysical Chemistry and Biomolecules

11591  [dx.doi.org/10.1021/jp505629q](https://doi.org/10.1021/jp505629q)

**Microscopic Hydration Properties of the  $A\beta_{1-42}$  Peptide Monomer and the Globular Protein Ubiquitin: A Comparative Molecular Dynamics Study**

Jaya C. Jose, Prabir Khatua, Nupur Bansal, Neelanjana Sengupta,\* and Sanjoy Bandyopadhyay\*

11605  [dx.doi.org/10.1021/jp506832u](https://doi.org/10.1021/jp506832u)

**SSB Binding to Single-Stranded DNA Probed Using Solid-State Nanopore Sensors**

Deanpen Japrunng, Azadeh Bahrami, Achim Nadzeyka, Lloyd Peto, Sven Bauerdick, Joshua B. Edel,\* and Tim Albrecht\*

11613 [dx.doi.org/10.1021/jp507062r](https://doi.org/10.1021/jp507062r)

**Local Water Dynamics around Antifreeze Protein Residues in the Presence of Osmolytes: The Importance of Hydroxyl and Disaccharide Groups**

Anand Narayanan Krishnamoorthy,\* Christian Holm, and Jens Smiatek\*

11622  [dx.doi.org/10.1021/jp507134y](https://doi.org/10.1021/jp507134y)

**Detecting a New Source for Photochemically Induced Dynamic Nuclear Polarization in the LOV2 Domain of Phototropin by Magnetic-Field Dependent  $^{13}\text{C}$  NMR Spectroscopy**

Gerd Kothe,\* Michail Lukaschek, Gerhard Link, Sylwia Kacprzak, Boris Illarionov, Markus Fischer, Wolfgang Eisenreich, Adelbert Bacher, and Stefan Weber\*

11633  [dx.doi.org/10.1021/jp507157e](https://doi.org/10.1021/jp507157e)

**All-Atom Molecular Dynamics Simulation of a Photosystem I/Detergent Complex**

Bradley J. Harris, Xiaolin Cheng, and Paul Frymier\*

11646  [dx.doi.org/10.1021/jp507270k](https://doi.org/10.1021/jp507270k)

**Chemical Modification of a Tetrapyrrole-Type Photosensitizer: Tuning Application and Photochemical Action beyond the Singlet Oxygen Channel**

Yasser M. Riyad,\* Sergej Naumov, Stanislaw Schastak, Jan Griebel, Axel Kahnt, Tilmann Häupl, Jochen Neuhaus, Bernd Abel, and Ralf Herrmann

11659 [dx.doi.org/10.1021/jp5075626](https://doi.org/10.1021/jp5075626)

**$\beta$ -Carotene As a Lipophilic Scavenger of Nitric Oxide**

Rui-Min Han, Hong Cheng, Ruopei Feng, Dan-Dan Li, Wenzhen Lai,\* Jian-Ping Zhang, and Leif H. Skibsted\*

11667  [dx.doi.org/10.1021/jp507902y](https://doi.org/10.1021/jp507902y)

**Effect of Functionalized Magnetic  $MnFe_2O_4$  Nanoparticles on Fibrillation of Human Serum Albumin**

Shubhatam Sen, Suraj Konar, Amita Pathak, Swagata Dasgupta,\* and Sunando DasGupta\*

11677  [dx.doi.org/10.1021/jp5079218](https://doi.org/10.1021/jp5079218)

**Protonation States of Remote Residues Affect Binding–Release Dynamics of the Ligand but Not the Conformation of Apo Ferric Binding Protein**

Gokce Guven, Ali Rana Atilgan, and Canan Atilgan\*

11688 [dx.doi.org/10.1021/jp508161s](https://doi.org/10.1021/jp508161s)

**Dissociation Pathways in the Cysteine Dication after Site-Selective Core Ionization**

J. Laksman,\* K. Kooser, H. Levola, E. Itälä, D. T. Ha, E. Rachlew, and E. Kukk

11696  [dx.doi.org/10.1021/jp508128d](https://doi.org/10.1021/jp508128d)

**Perturbation of Long-Range Water Dynamics as the Mechanism for the Antifreeze Activity of Antifreeze Glycoprotein**

Sairam S. Mallajosyula, Kenno Vanommeslaeghe, and Alexander D. MacKerell Jr.\*

11707  [dx.doi.org/10.1021/jp5082017](https://doi.org/10.1021/jp5082017)

**pH-Related and Site-Specific Excited-State Proton Transfer from Pterin to Acetate**

Lei Liu, Dapeng Yang, and Peng Li\*

**Biomaterials, Surfactants, and Membranes**

11715 [dx.doi.org/10.1021/jp5022278](https://doi.org/10.1021/jp5022278)

**Pulsed Magnetic Field Induced Fast Drug Release from Magneto Liposomes via Ultrasound Generation**

George Podaru, Saralyn Ogden, Amanda Baxter, Tej Shrestha, Shengqiang Ren, Prem Thapa, Raj Kumar Dani, Hongwang Wang, Matthew T. Basel, Punit Prakash, Stefan H. Bossmann,\* and Viktor Chikan

11723  [dx.doi.org/10.1021/jp5050892](https://doi.org/10.1021/jp5050892)

**Molecular Dynamics Simulations of DPPC/CTAB Monolayers at the Air/Water Interface**

Bin Liu, Matthew I. Hoopes, and Mikko Karttunen\*

11738

[dx.doi.org/10.1021/jp5055765](https://doi.org/10.1021/jp5055765)**Magnetic Nanoparticles for in Vivo Use: A Critical Assessment of Their Composition**

Geraldo Magela da Costa, Cristina Blanco-Andujar, Eddy De Grave, and Quentin A. Pankhurst\*

11747

[dx.doi.org/10.1021/jp508841p](https://doi.org/10.1021/jp508841p)**From Material Science to Avant-Garde Cuisine. The Art of Shaping Liquids into Spheres**

Haohao Fu, Yingzhe Liu, Ferran Adria, Xueguang Shao, Wensheng Cai,\* and Christophe Chipot\*

**Liquids; Chemical and Dynamical Processes in Solution**

11757

[dx.doi.org/10.1021/jp505147u](https://doi.org/10.1021/jp505147u)**Molecular Dynamics Simulation of Aqueous Urea Solution: Is Urea a Structure Breaker?**

Dibyendu Bandyopadhyay, Sadhana Mohan, Swapan K. Ghosh, and Niharendu Choudhury\*

11769

[dx.doi.org/10.1021/jp505731z](https://doi.org/10.1021/jp505731z)**Prediction of Cosolvent Effect on Solvation Free Energies and Solubilities of Organic Compounds in Supercritical Carbon Dioxide Based on Fully Atomistic Molecular Simulations**

Andrey I. Frolov\* and Michael G. Kiselev

11781

[dx.doi.org/10.1021/jp506326u](https://doi.org/10.1021/jp506326u)**Dynamics of Ground and Excited State Vibrational Relaxation and Energy Transfer in Transition Metal Carbonyls**

Milan Delor, Igor V. Sazanovich, Michael Towrie, Steven J. Spall, Theo Keane, Alexander J. Blake, Claire Wilson, Anthony J. H. M. Meijer,\* and Julia A. Weinstein\*

11792

[dx.doi.org/10.1021/jp5079696](https://doi.org/10.1021/jp5079696)**Viscosity of Fluid Nitrogen to Pressures of 10 GPa**

Evan H. Abramson\*

11797

[dx.doi.org/10.1021/jp507978u](https://doi.org/10.1021/jp507978u)**Dissociation of Methane Hydrate in Aqueous NaCl Solutions**

Takuma Yagasaki, Masakazu Matsumoto, Yoshimichi Andoh, Susumu Okazaki, and Hideki Tanaka\*

**Glasses, Colloids, Polymers, and Soft Matter**

11805

[dx.doi.org/10.1021/jp504175f](https://doi.org/10.1021/jp504175f)**DNA Assisted Self-Assembly of PAMAM Dendrimers**

Taraknath Mandal, Mattaparthi Venkata Satish Kumar, and Prabal K. Maiti\*

11816

[dx.doi.org/10.1021/jp504217m](https://doi.org/10.1021/jp504217m)**Structure and Rheology of Mixed Suspensions of Montmorillonite and Silica Nanoparticles**

Jan Hilhorst,\* Vera Meester, Esther Groeneveld, Jan K. G. Dhont, and Henk N. W. Lekkerkerker

**Size Selectivity in the Confined Ternary Colloidal Mixtures: The Depletion in the Competition**

Zongli Sun,\* Yanshuang Kang, and Yanmei Kang

11835

dx.doi.org/10.1021/jp507230m

**Interactions of Small Dendrimers with Sodium Dodecyl Sulfate at the Air–Water Interface**

Marianna Yanez Arteta,\* Richard A. Campbell, Erik B. Watkins, Marc Obiols-Rabasa, Karin Schillén, and Tommy Nylander\*

11849

dx.doi.org/10.1021/jp5074279

**Polarization Holograms in a Bifunctional Amorphous Polymer Exhibiting Equal Values of Photoinduced Linear and Circular Birefringences**

Clementina Provenzano,\* Pasquale Pagliusi, Gabriella Cipparrone, Jorge Royes, Milagros Piñol, and Luis Oriol

11855 **S**

dx.doi.org/10.1021/jp5077005

**Rydberg and  $\pi$ – $\pi^*$  Transitions in Film Surfaces of Various Kinds of Nylons Studied by Attenuated Total Reflection Far-Ultraviolet Spectroscopy and Quantum Chemical Calculations: Peak Shifts in the Spectra and Their Relation to Nylon Structure and Hydrogen Bondings**

Yusuke Morisawa,\* Manaka Yasunaga, Harumi Sato, Ryoichi Fukuda, Masahiro Ehara,\* and Yukihiko Ozaki

## Additions and Corrections

11862

dx.doi.org/10.1021/jp509310h

**Correction to “Phase Structure and Phase Transition Mechanism for Light-Induced *1a3d* Cubic Phase in 4′-*n*-Docosyloxy-3′-nitrophenyl-4-carboxylic acid/Ethyl 4-(4′-*n*-Docosyloxyphenylazo)benzoate Binary Mixture”**

Ryo Hori, Yohei Miwa,\* Katsuhiro Yamamoto, and Shoichi Kutsumizu