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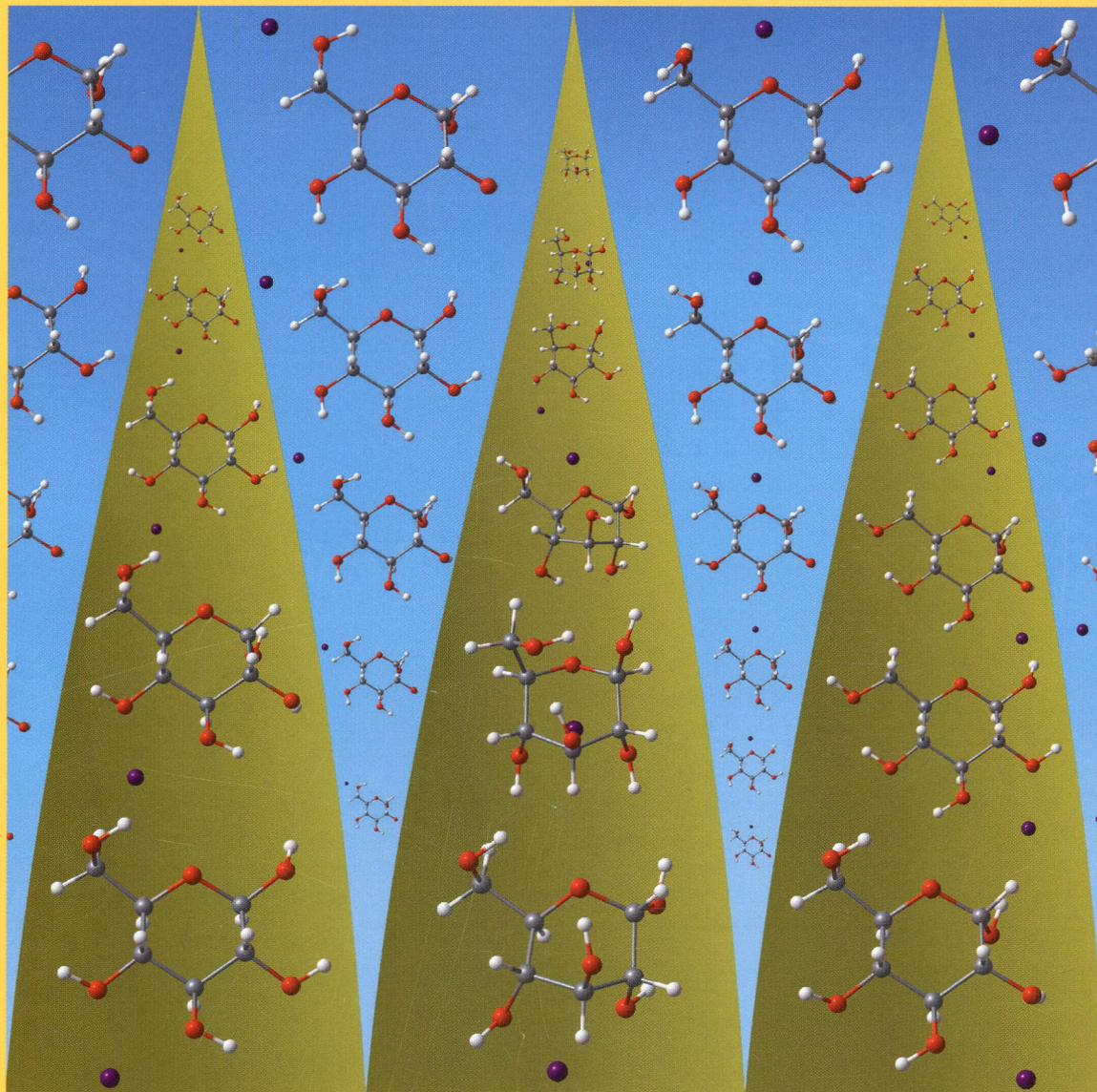
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# THE JOURNAL OF PHYSICAL CHEMISTRY

# B



Promiscuous Sodium  
Ion Binding with  
Aqueous  $\alpha$ - and  
 $\beta$ -Glucose  
(see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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**ON THE COVER:** Promiscuous sodium ion binding with aqueous  $\alpha$ - and  $\beta$ -glucose. Quantum mechanics and molecular dynamics have elucidated the many low-energy conformations wherein a sodium ion interacts with  $\alpha$ - and  $\beta$ -glucose and the ion's effect on electronic and geometric properties. Experiment further provides the first quantitative data showing how the presence of NaCl affects the ratio of the anomeric populations of this important monosaccharide. This work provides a solid foundation for mechanistic understanding of how these interactions affect the reactivity of systems of interest for sustainable chemistry. See page 1990.

## Articles

### Biophysical Chemistry and Biomolecules

1969

dx.doi.org/10.1021/jp401072k

**Proton Transfer Pathways, Energy Landscape, and Kinetics in Creatine–Water Systems**

Olga Ivchenko,\* Chris S. Whittleston, Joanne M. Carr, Petra Imhof, Steffen Goerke, Peter Bachert, and David J. Wales\*

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**Theoretical and Experimental Studies on Activity of *Yarrowia lipolytica* Lipase in Methanol/Water Mixtures**

Lingli Li, Yang Jiang, Haiyang Zhang, Wei Feng, Biqiang Chen, and Tianwei Tan\*

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dx.doi.org/10.1021/jp407379t

**Electrophoretic Mobilities of a Viral Capsid, Its Capsid Protein, and Their Relation to Viral Assembly**

J. R. Vega-Acosta, R. D. Cadena-Nava, W. M. Gelbart, C. M. Knobler,\* and J. Ruiz-García\*

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**Sodium Ion Interactions with Aqueous Glucose: Insights from Quantum Mechanics, Molecular Dynamics, and Experiment**

Heather B. Mayes, Jianhui Tian, Michael W. Nolte, Brent H. Shanks, Gregg T. Beckham, S. Gnanakaran,\* and Linda J. Broadbelt\*

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Yu-Jiao Chen, Ning Deng, Bin Hu, Yan Wang, and Jian-Bo He\*

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**Catalytic Mechanism of Histone Acetyltransferase p300: From the Proton Transfer to Acetylation Reaction**

Xinlei Zhang, Sisheng Ouyang, Xiangqian Kong, Zhongjie Liang, Junyan Lu, Kongkai Zhu, Dan Zhao, Mingyue Zheng, Hualiang Jiang, Xin Liu, Ronen Marmorstein, and Cheng Luo\*

- 2020  [dx.doi.org/10.1021/jp4103349](https://doi.org/10.1021/jp4103349)  
**Measurement and Control of pH in the Aqueous Interior of Reverse Micelles**  
Bryan S. Marques, Nathaniel V. Nucci, Igor Dodevski, Kristina W. C. Wang, Evangelia A. Athanasoula, Christine Jorge, and A. Joshua Wand\*
- 2032  [dx.doi.org/10.1021/jp410586f](https://doi.org/10.1021/jp410586f)  
**Modeling of Various Optical Spectra in the Presence of Slow Excitation Energy Transfer in Dimers and Trimers with Weak Interpigment Coupling: FMO as an Example**  
Nicoleta Herascu, Adam Kell, Khem Acharya, Ryszard Jankowiak,\* Robert E. Blankenship, and Valter Zazubovich\*
- 2041  [dx.doi.org/10.1021/jp4107537](https://doi.org/10.1021/jp4107537)  
**Molecular Strategies to Achieve Selective Conductance in NaK Channel Variants**  
Yibo Wang, Adam C. Chamberlin, and Sergei Yu. Noskov\*
- 2050  [dx.doi.org/10.1021/jp410788r](https://doi.org/10.1021/jp410788r)  
**Effects of Branched O-Glycosylation on a Semiflexible Peptide Linker**  
Quentin R. Johnson, Richard J. Lindsay, Sherin R. Raval, Jeremy S. Dobbs, Ricky B. Nellas, and Tongye Shen\*
- 2058  [dx.doi.org/10.1021/jp411020a](https://doi.org/10.1021/jp411020a)  
**Intensity Dependence of the Excited State Lifetimes and Triplet Conversion Yield in the Fenna–Matthews–Olson Antenna Protein**  
Gregory S. Orf, Dariusz M. Niedzwiedzki, and Robert E. Blankenship\*
- 2070  [dx.doi.org/10.1021/jp411476p](https://doi.org/10.1021/jp411476p)  
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Yu Wang,\* Yuhei Hayamizu, and Hidefumi Akiyama
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Jasmeet Singh and Radha Ranganathan\*
- 2084  [dx.doi.org/10.1021/jp412538n](https://doi.org/10.1021/jp412538n)  
**Effect of Protein Environment within Cytochrome P450cam Evaluated Using a Polarizable-Embedding QM/MM Method**  
Nandun M. Thellamurege and Hajime Hirao\*
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**Exploring the Conformational Space of Cysteine by Matrix Isolation Spectroscopy Combined with Near-Infrared Laser Induced Conformational Change**  
Eszter E. Najbauer, Gábor Bazsó, Sándor Góbi, Gábor Magyarfalvi, and György Tarczay\*

## Biomaterials, Surfactants, and Membranes

2104  [dx.doi.org/10.1021/jp4114317](https://doi.org/10.1021/jp4114317)  
**Induced Crystallization of Amorphous Biosilica to Cristobalite by Silicic acid**  
Ido Fuchs, Yaniv Aluma, Micha Ilan, and Yitzhak Mastai\*

2112  [dx.doi.org/10.1021/jp4124315](https://doi.org/10.1021/jp4124315)  
**Detergent Induction of HEK 293A Cell Membrane Permeability Measured under Quiescent and Superfusion Conditions Using Whole Cell Patch Clamp**  
Sriram Vaidyanathan, Bradford G. Orr, and Mark M. Banaszak Holl\*

2124 [dx.doi.org/10.1021/jp500316s](https://doi.org/10.1021/jp500316s)  
**Secondary Structure, Backbone Dynamics, and Structural Topology of Phospholamban and Its Phosphorylated and Arg9Cys-Mutated Forms in Phospholipid Bilayers Utilizing  $^{13}\text{C}$  and  $^{15}\text{N}$  Solid-State NMR Spectroscopy**  
Xueting Yu and Gary A. Lorigan\*

## Liquids; Chemical and Dynamical Processes in Solution

2134  [dx.doi.org/10.1021/jp4105272](https://doi.org/10.1021/jp4105272)  
**NMR Investigation of Chloromethane Complexes of Cryptophane-A and Its Analogue with Butoxy Groups**  
Z. Takacs, E. Steiner, J. Kowalewski,\* and T. Brotin

2147 [dx.doi.org/10.1021/jp411363d](https://doi.org/10.1021/jp411363d)  
**Physical Nature of Intermolecular Interactions in [BMIM][PF<sub>6</sub>] Ionic Liquid**  
Borys Szefczyk\* and W. Andrzej Sokalski

2157  [dx.doi.org/10.1021/jp411471r](https://doi.org/10.1021/jp411471r)  
**Diffusion of Squalene in *n*-Alkanes and Squalane**  
Bruce A. Kowert,\* Michael B. Watson, and Nhan C. Dang

2164 [dx.doi.org/10.1021/jp412090k](https://doi.org/10.1021/jp412090k)  
**Pressure Tuning of Electron Attachment to Benzoquinones in Nonpolar Fluids: Continuous Adjustment of Free Energy Changes**  
Richard Holroyd,\* John R. Miller,\* Andrew R. Cook,\* and Masaru Nishikawa

2172 [dx.doi.org/10.1021/jp412330u](https://doi.org/10.1021/jp412330u)  
**The Molar Volumes of Ions in Solution, Part 7. Electrostriction and Hydration Numbers of Aqueous Polyatomic Anions at 25 °C**  
Yizhak Marcus\*

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**Cation and Anion Transport in a Dicationic Imidazolium-Based Plastic Crystal Ion Conductor**  
Bryce E. Kidd, Mark D. Lingwood, Minjae Lee, Harry W. Gibson, and Louis A. Madsen\*
- 2186 dx.doi.org/10.1021/jp410604a  
**Influence of Magnetic Nanoparticle Size on the Particle Dispersion and Phase Separation in an ABA Triblock Copolymer**  
Jinrong Wu, Hui Li, Siduo Wu, Guangsu Huang,\* Wang Xing, Maozhu Tang, and Qiang Fu\*
- 2194 dx.doi.org/10.1021/jp410983x  
**Internal Structures of Thermosensitive Hybrid Microgels Investigated by Means of Small-Angle X-ray Scattering**  
Daisuke Suzuki,\* Yasuhisa Nagase, Takuma Kureha, and Takaaki Sato
- 2205 dx.doi.org/10.1021/jp411204b  
**EPR Study of Polyaniline Synthesized Enzymatically in the Presence of Submicrometer-Sized AOT Vesicles**  
Boris Rakvin,\* Dejana Carić, Mladen Andreis, Katja Junker, and Peter Walde
- 2214 dx.doi.org/10.1021/jp4112712  
**Nanoparticle-Driven Intermolecular Cooperativity and Miscibility in Polystyrene/Poly(vinyl methyl ether) Blends**  
Avanish Bharati, Priti Xavier, Goutam Prasanna Kar, Giridhar Madras, and Suryasarathi Bose\*
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**Appearance of Perfect Amorphous Linear Bulk Polyethylene under Applied Electric Field and the Analysis by Radial Distribution Function and Direct Tunneling Effect**  
Rong Zhang, Yuezhen Bin, Wenxiao Yang, Shaoyan Fan, and Masaru Matsuo\*
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**Comparative Analysis of Fluorine-Containing Mesogenic Derivatives of Carborane, Bicyclo[2.2.2]octane, Cyclohexane, and Benzene using the Maier–Meier Theory**  
Piotr Kaszynski,\* Adam Januszko, and Kristin L. Glab
- 2249 dx.doi.org/10.1021/jp411823j  
**Topological Origin of Fragility, Network Adaptation, and Rigidity and Stress Transitions in Especially Homogenized Nonstoichiometric Binary  $\text{Ge}_x\text{S}_{100-x}$  Glasses**  
Shibalik Chakraborty and P. Boolchand\*
- 2264 dx.doi.org/10.1021/jp412229j  
**Combined SAXS/UV–vis/Raman as a Diagnostic and Structure Resolving Tool in Materials and Life Sciences Applications**  
Sylvio Haas,\* Tomás S. Plivelic,\* and Cedric Dicko

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**Thermoregulated Formation and Disintegration of Cationic Block Copolymer Vesicles: Fluorescence Resonance Energy Transfer Study**

Chiranjit Maiti, Debabrata Dey, Sarthak Mandal, and Dibakar Dhara\*

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[dx.doi.org/10.1021/jp412451h](https://doi.org/10.1021/jp412451h)

**Structural and Topological Control on Physical Properties of Arsenic Selenide Glasses**

Derrick C. Kaseman, Ivan Hung, Zhehong Gan, Bruce Aitken, Steven Currie, and Sabyasachi Sen\*