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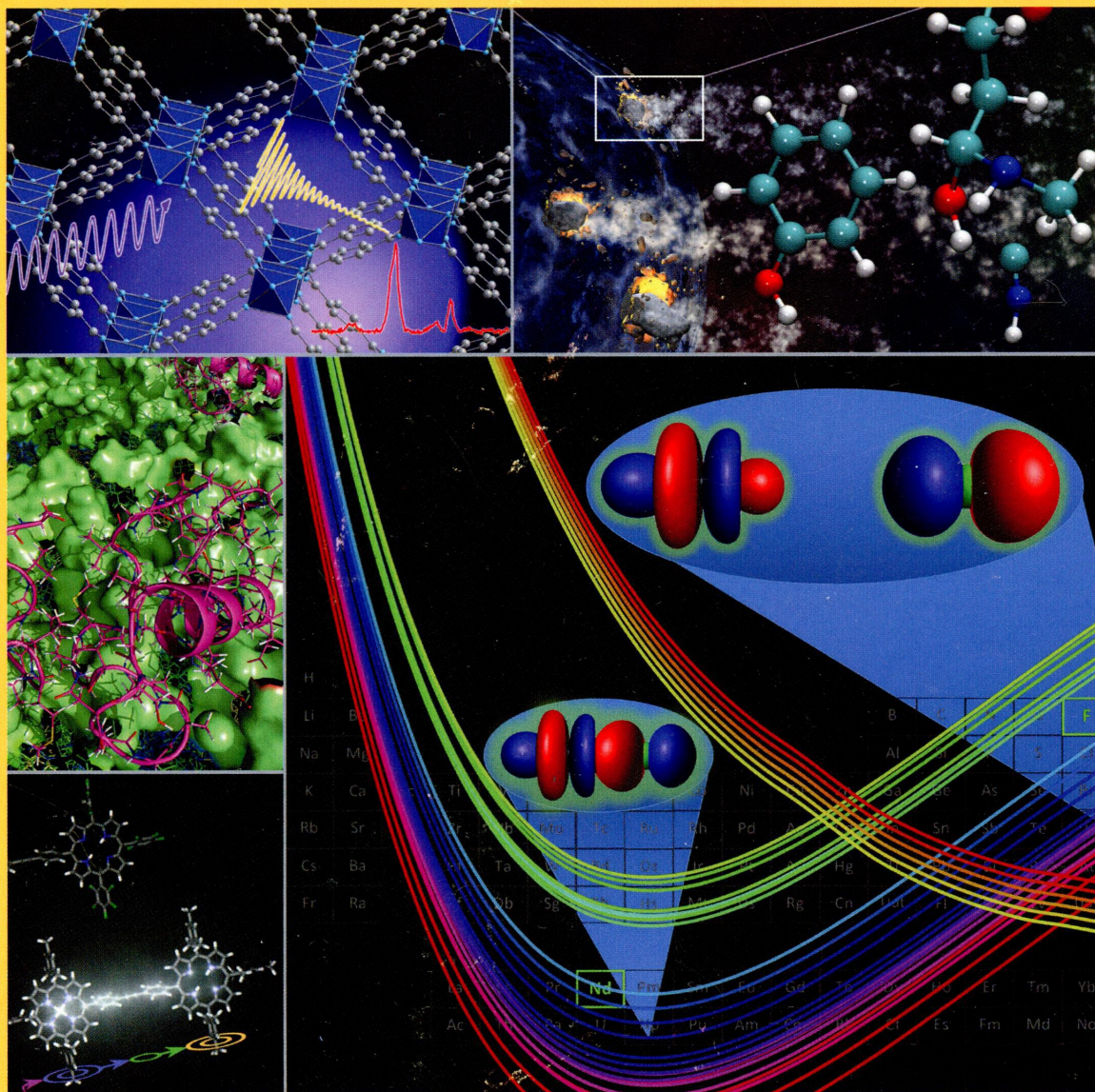
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# THE JOURNAL OF PHYSICAL CHEMISTRY

B



**BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER**



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**ON THE COVER:** Collage of cover art from recent issues of *J. Phys. Chem.* Top Left:  $^{17}\text{O}$  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  $\beta$ -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  $\text{NdF}^{2+}$  (*J. Phys. Chem. A* **2013**, *117* (42), 10881–10888).

## Articles

### Biophysical Chemistry and Biomolecules

10553



dx.doi.org/10.1021/jp502852f

#### Single Water Entropy: Hydrophobic Crossover and Application to Drug Binding

Wilbee D. Sasikala and Arnab Mukherjee\*

10565



dx.doi.org/10.1021/jp504133m

#### Sodium Dodecyl Sulfate Monomers Induce XAO Peptide Polyproline II to $\alpha$ -Helix Transition

Zhenmin Hong, Krishnan Damodaran, and Sanford A. Asher\*

10576



dx.doi.org/10.1021/jp504820w

#### Exploring Regions of Conformational Space Occupied by Two-Domain Proteins

Witold Andrajoć, Claudio Luchinat,\* Giacomo Parigi, and Enrico Ravera

10588

dx.doi.org/10.1021/jp505179h

#### Importance of Excitation and Trapping Conditions in Photosynthetic Environment-Assisted Energy Transport

Roberto de J. León-Montiel,\* Ivan Kassal, and Juan P. Torres

10595



dx.doi.org/10.1021/jp505295j

#### Kinetic Analysis of the Multistep Aggregation Mechanism of Monoclonal Antibodies

Lucrece Nicoud, Paolo Arosio, Margaux Sozo, Andrew Yates, Edith Norrant, and Massimo Morbidelli\*

10607



dx.doi.org/10.1021/jp505938t

#### Characterizing Solution Surface Loop Conformational Flexibility of the GM2 Activator Protein


Jeffery D. Carter, Jordan D. Mathias, Edwin F. Gomez, Yong Ran, Fang Xu, Luis Galiano, Nguyen Q. Tran, Peter W. D'Amore, Christine S. Wright, Dhruva K. Chakravorty, and Gail E. Fanucci\*

10618 

[dx.doi.org/10.1021/jp506379r](https://doi.org/10.1021/jp506379r)

**Modeling the Solvation of Nonpolar Amino Acids in Guanidinium Chloride Solutions**

Paul Cohen, Ken A. Dill, and Sheila S. Jaswal\*

10624 

[dx.doi.org/10.1021/jp506594f](https://doi.org/10.1021/jp506594f)

**Interactions of Macromolecular Crowding Agents and Cosolutes with Small-Molecule Substrates: Effect on Horseradish Peroxidase Activity with Two Different Substrates**

William M. Aumiller Jr., Bradley W. Davis, Emmanuel Hatzakis, and Christine D. Keating\*

**Biomaterials, Surfactants, and Membranes**

10633

[dx.doi.org/10.1021/jp504526f](https://doi.org/10.1021/jp504526f)

**Gemini Surfactants Affect the Structure, Stability, and Activity of Ribonuclease Sa**

Razieh Amiri, Abdol-Khalegh Bordbar, and Douglas V. Laurents\*

10643

[dx.doi.org/10.1021/jp5053419](https://doi.org/10.1021/jp5053419)

**Coarse-Grained Computational Studies of Supported Bilayers: Current Problems and Their Root Causes**

Antti Lamberg and Takashi Taniguchi\*

10653 

[dx.doi.org/10.1021/jp505657x](https://doi.org/10.1021/jp505657x)

**Correlation of [RuCl<sub>3</sub>(dppb)(VPy)] Cytotoxicity with its Effects on the Cell Membranes: An Investigation Using Langmuir Monolayers as Membrane Models**


B. Sandrino,\* T. T. Tominaga, T. M. Nobre, L. Scorsin, E. C. Wrobel, B. C. Fiorin, M. P. de Araujo, L. Caseli, O. N. Oliveira Jr., and K. Wohnrath\*

10662 

[dx.doi.org/10.1021/jp505661e](https://doi.org/10.1021/jp505661e)

**Observation of a Rare Earth Ion–Extractant Complex Arrested at the Oil–Water Interface During Solvent Extraction**

Wei Bu,\* Hao Yu, Guangming Luo, Mrinal K. Bera, Binyang Hou, Adam W. Schuman, Binhua Lin, Mati Meron, Ivan Kuzmenko, Mark R. Antonio, L. Soderholm,\* and Mark L. Schlossman\*

10675 

[dx.doi.org/10.1021/jp5059319](https://doi.org/10.1021/jp5059319)

**Understanding Solvation in the Low Global Warming Hydrofluoroolefin HFO-1234ze Propellant**

Lin Yang and Sandro R. P. da Rocha\*

10688 

[dx.doi.org/10.1021/jp506096h](https://doi.org/10.1021/jp506096h)

**Emergence of DNA-Encapsulating Liposomes from a DNA–Lipid Blend Film**


Shunsuke F. Shimobayashi\* and Masatoshi Ichikawa\*

10695

[dx.doi.org/10.1021/jp506768b](https://doi.org/10.1021/jp506768b)

**Surface–Bulk Partition of Surfactants Predicted by Molecular Dynamics Simulations**

Chunwei Yang and Huai Sun\*

10704 

[dx.doi.org/10.1021/jp506885r](https://doi.org/10.1021/jp506885r)

**Observation of the Marcus Inverted Region for Bimolecular Photoinduced Electron-Transfer Reactions in Viscous Media**  
Manoj Kumbhakar,\* Arpan Manna, Mhejabeen Sayed, Anil Kumar, and Haridas Pal\*

## Liquids; Chemical and Dynamical Processes in Solution

10716 

[dx.doi.org/10.1021/jp5054875](https://doi.org/10.1021/jp5054875)


**Atomistic Force Field for Pyridinium-Based Ionic Liquids: Reliable Transport Properties**  
Iuliia V. Voroshylova\* and Vitaly V. Chaban

## Glasses, Colloids, Polymers, and Soft Matter

10725


[dx.doi.org/10.1021/jp5023168](https://doi.org/10.1021/jp5023168)

**Charging and Uncharging a Neutral Polymer in Solution: A Small-Angle Neutron Scattering Investigation**  
Ankitkumar I. Fajalia and Marina Tsianou\*

10740 

[dx.doi.org/10.1021/jp502806v](https://doi.org/10.1021/jp502806v)

**Form Factor of Asymmetric Elongated Micelles: Playing with Russian Dolls Has Never Been so Informative**  
Gerald Guerin, Graeme Cambridge, Mohsen Soleimani, Sepehr Mastour Tehrani, Ian Manners,\* and Mitchell A. Winnik\*

10750 

[dx.doi.org/10.1021/jp5040135](https://doi.org/10.1021/jp5040135)

**Molecular Dynamics Simulations of Tri-*n*-butyl-phosphate/*n*-Dodecane Mixture: Thermophysical Properties and Molecular Structure**  
Shengting Cui,\* Valmor F. de Almeida, and Bamin Khomami\*

10761

[dx.doi.org/10.1021/jp504537n](https://doi.org/10.1021/jp504537n)

**Structural Properties of Dense Hard Sphere Packings**  
Boris A. Klumov,\* Yuliang Jin, and Hernán A. Makse

10767 

[dx.doi.org/10.1021/jp504585k](https://doi.org/10.1021/jp504585k)

**NMR and Molecular Dynamics Study of the Size, Shape, and Composition of Reverse Micelles in a Cetyltrimethylammonium Bromide (CTAB)/*n*-Hexane/Pentanol/Water Microemulsion**  
Amanda J. Mills, John Wilkie, and Melanie M. Britton\*

10776

[dx.doi.org/10.1021/jp5062368](https://doi.org/10.1021/jp5062368)

**Phase Separation of Aqueous Poly(2-dimethylaminoethyl methacrylate-*block*-*N*-vinylcaprolactams)**  
Mikko Karesoja,\* Erno Karjalainen, Sami Hietala, and Heikki Tenhu\*

10785 

[dx.doi.org/10.1021/jp506422p](https://doi.org/10.1021/jp506422p)

**Structure and Energetics of  $\text{Li}^+(\text{BF}_4^-)_n$ ,  $\text{Li}^+(\text{FSI}^-)_n$ , and  $\text{Li}^+(\text{TFSI}^-)_n$ : Ab Initio and Polarizable Force Field Approaches**  
Charles W. Bauschlicher Jr.,\* Justin B. Haskins, Eric W. Bucholz, John W. Lawson, and Oleg Borodin

10795

[dx.doi.org/10.1021/jp506782d](https://doi.org/10.1021/jp506782d)

**Evaluation of Growth Front Velocity in Ultrastable Glasses of Indomethacin over a Wide Temperature Interval**

Cristian Rodríguez-Tinoco, Marta Gonzalez-Silveira,\* Joan Ràfols-Ribé, Aitor F. Lopeandia, Maria Teresa Clavaguera-Mora, and Javier Rodríguez-Viejo\*

## Comments

10802

[dx.doi.org/10.1021/jp508089t](https://doi.org/10.1021/jp508089t)

**Comment on "Hydration and Mobility of Trehalose in Aqueous Solution"**

M. Heyden,\* G. Schwaab, and M. Havenith

10806



[dx.doi.org/10.1021/jp5083467](https://doi.org/10.1021/jp5083467)

**Reply to "Comment on 'Hydration and Mobility of Trehalose in Aqueous Solution'"**

Bertil Halle\*