

JANUARY 8, 2015

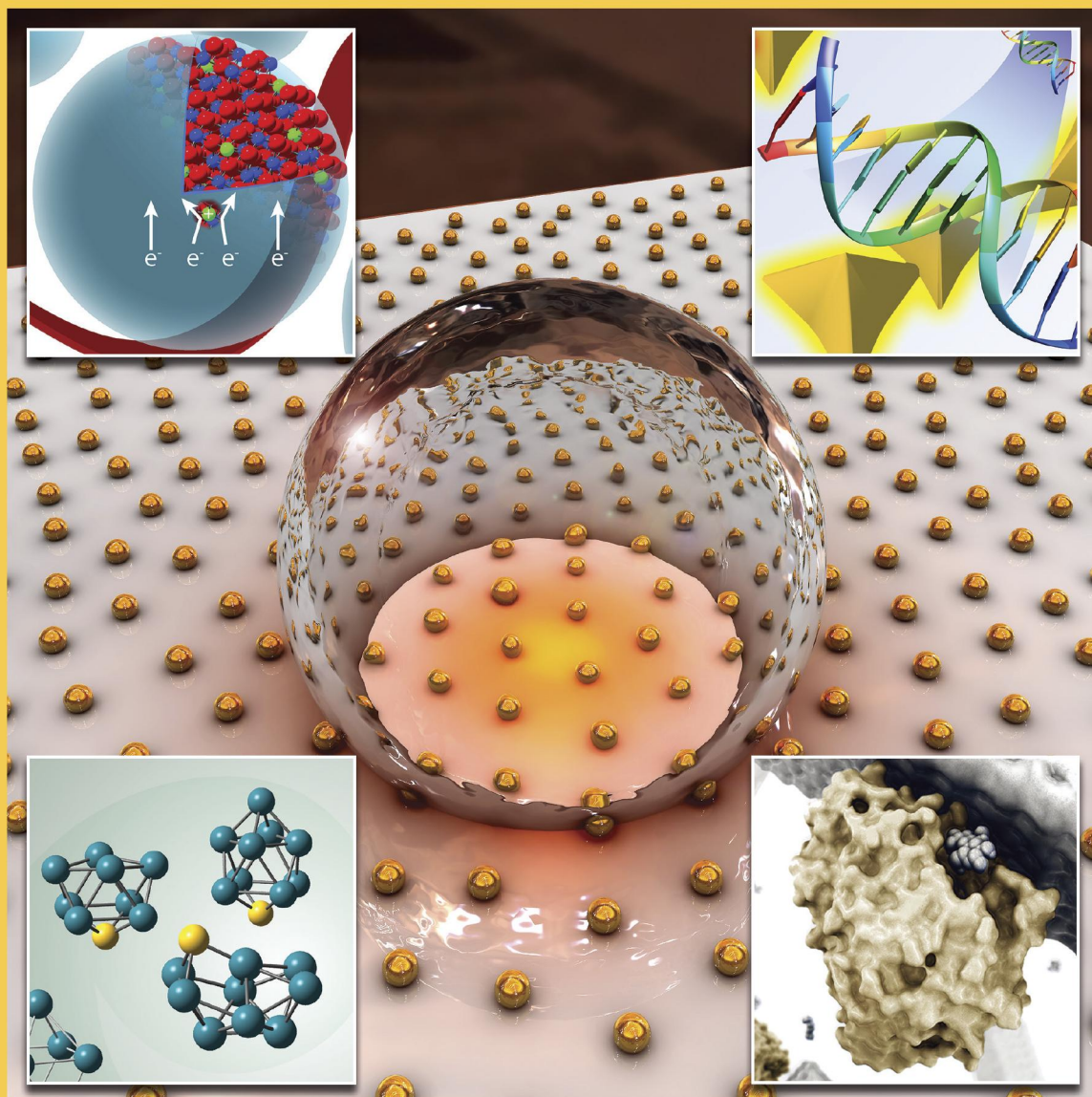
VOLUME 119

NUMBER 1

[pubs.acs.org/JPCB](http://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](http://www.acs.org)

January 8, 2015: Vol. 119, Iss. 1

## Content

### 1. Editorial for January 2015 for JPC A/B/C

Anne B. McCoy, Joan-Emma Shea, Catherine J. Murphy, and George C. Schatz  
*The Journal of Physical Chemistry B* 2015 119 (1), 1-4

### 2. Ligand 5,10,15,20-Tetra(N-methyl-4-pyridyl)porphine (TMPyP4) Prefers the Parallel Propeller-Type Human Telomeric G-Quadruplex DNA over Its Other Polymorphs

Asfa Ali, Manju Bansal, and Santanu Bhattacharya  
*The Journal of Physical Chemistry B* 2015 119 (1), 5-14

### 3. Molecular Mechanism of the Inhibition and Remodeling of Human Islet Amyloid Polypeptide (hIAPP1–37) Oligomer by Resveratrol from Molecular Dynamics Simulation

Qianqian Wang, Lulu Ning, Yuzhen Niu, Huanxiang Liu, and Xiaojun Yao  
*The Journal of Physical Chemistry B* 2015 119 (1), 15-24

### 4. AFM-Based Quantification of Conformational Changes in DNA Caused by Reactive Oxygen Species

Florian Berg, Janine Wilken, Christiane A. Helm, and Stephan Block  
*The Journal of Physical Chemistry B* 2015 119 (1), 25-32

### 5. Coulomb Repulsion in Short Polypeptides

Amir Norouzy, Khaleel I. Assaf, Shuai Zhang, Maik H. Jacob, and Werner M. Nau  
*The Journal of Physical Chemistry B* 2015 119 (1), 33-43

### 6. Activation Kinetics of Zipper Molecular Beacons

Tracy W. Liu, Juan Chen, Laura Burgess, Brian C. Wilson, Gang Zheng, Lixin Zhan, Wing-Ki Liu, and Bae-Yeun Ha  
*The Journal of Physical Chemistry B* 2015 119 (1), 44-53

### 7. Side-Chain Packing Interactions Stabilize an Intermediate of BAX Protein against Chemical and Thermal Denaturation

Chun-Hui Chan, Chia-Jung Tsai, and Yun-Wei Chiang  
*The Journal of Physical Chemistry B* 2015 119 (1), 54-64

## **8. Thermodynamic Investigations of [(phen)<sub>2</sub>Ru(tatpp)Ru(phen)<sub>2</sub>]<sup>4+</sup> Interactions with B-DNA**

Vu H. Le, Matthew R. McGuire, Pooja Ahuja, Frederick M. MacDonnell, and Edwin A. Lewis  
*The Journal of Physical Chemistry B* **2015** 119 (1), 65-71

## **9. Determination of Conformational Entropy of Fully and Partially Folded Conformations of Holo- and Apomyoglobin**

Andreas M. Stadler, Michael Marek Koza, and Jörg Fitter  
*The Journal of Physical Chemistry B* **2015** 119 (1), 72-82

## **10. Understanding Zinc(II) Chelation with Quercetin and Luteolin: A Combined NMR and Theoretical Study**

Alexandra Primikyri, Gloria Mazzone, Christina Lekka, Andreas G. Tzakos, Nino Russo, and Ioannis P. Gerothanassis  
*The Journal of Physical Chemistry B* **2015** 119 (1), 83-95

## **11. The Size of the Internal Loop in DNA Hairpins Influences Their Targeting with Partially Complementary Strands**

Iztok Prislán, Hui-Ting Lee, Cynthia Lee, and Luis A. Marky  
*The Journal of Physical Chemistry B* **2015** 119 (1), 96-104

## **12. Multiscale Simulations of Human Telomeric G-Quadruplex DNA**

Matúš Rebič, Francesca Mocchi, Aatto Laaksonen, and Jozef Uličný  
*The Journal of Physical Chemistry B* **2015** 119 (1), 105-113

## **13. Molecular Dynamics Simulations of Heart-type Fatty Acid Binding Protein in Apo and Holo Forms, and Hydration Structure Analyses in the Binding Cavity**

Daisuke Matsuoka, Shigeru Sugiyama, Michio Murata, and Shigeru Matsuoka  
*The Journal of Physical Chemistry B* **2015** 119 (1), 114-127

## **14. Solvation and Hydration of the Ceramide Headgroup in a Non-Polar Solution**

Richard J. Gillams, Jon V. Busto, Sebastian Busch, Félix M. Goñi, Christian D. Lorenz, and Sylvia E. McLain  
*The Journal of Physical Chemistry B* **2015** 119 (1), 128-139

## **15. Modulation of the Rate of Reversible Electron Transfer in Oxidized Tryptophan and Tyrosine Containing Peptides in Acidic Aqueous Solution**

Olga B. Morozova and Alexandra V. Yurkovskaya  
*The Journal of Physical Chemistry B* **2015** 119 (1), 140-149

## **16. Synergy in Protein–Osmolyte Mixtures**

Jörg Rösgen

*The Journal of Physical Chemistry B* **2015** 119 (1), 150-157

## **17. Time to Overcome the High, Long, and Bumpy Free Energy Barrier in a Multi-Stage Process: The Generalized Steady-State Approach**

Alexei V. Finkelstein

*The Journal of Physical Chemistry B* **2015** 119 (1), 158-163

## **18. Protein Denaturants at Aqueous–Hydrophobic Interfaces: Self-Consistent Correlation between Induced Interfacial Fluctuations and Denaturant Stability at the Interface**

Di Cui, Shu-Ching Ou, and Sandeep Patel

*The Journal of Physical Chemistry B* **2015** 119 (1), 164-178

## **19. Amphiphile Micelle Structures in the Protic Ionic Liquid Ethylammonium Nitrate and Water**

Zhengfei Chen, Tamar L. Greaves, Rachel A. Caruso, and Calum J. Drummond

*The Journal of Physical Chemistry B* **2015** 119 (1), 179-191

## **20. Electroporation Threshold of POPC Lipid Bilayers with Incorporated Polyoxyethylene Glycol (C12E8)**

Andraž Polak, Aljaž Velikonja, Peter Kramar, Mounir Tarek, and Damijan Miklavčič

*The Journal of Physical Chemistry B* **2015** 119 (1), 192-200

## **21. Predominant Role of Water in Native Collagen Assembly inside the Bone Matrix**

Ratan Kumar Rai, Chandan Singh, and Neeraj Sinha

*The Journal of Physical Chemistry B* **2015** 119 (1), 201-211

## **22. Understanding Nitric Acid-Induced Changes in the Arrangement of Monomeric and Polymeric Methacryloyl Diglycolamides on Their Affinity toward f-Element Ions**

Vivek Chavan, Sabyasachi Patra, Ashok K. Pandey, Vasudevan Thekkethil, Mudassir Iqbal,

Jurriaan Huskens, Debasis Sen, S. Mazumder, Asok Goswami, and Willem Verboom

*The Journal of Physical Chemistry B* **2015** 119 (1), 212-218

## **23. Multisite Ion Model in Concentrated Solutions of Divalent Cations (MgCl<sub>2</sub> and CaCl<sub>2</sub>): Osmotic Pressure Calculations**

Akansha Saxena and Angel E. García

*The Journal of Physical Chemistry B* **2015** 119 (1), 219-227

## **24. Electrohydrodynamic Flow through a 1 mm<sup>2</sup> Cross-Section Pore Placed in an Ion-Exchange Membrane**

Kentaro Doi, Ayako Yano, and Satoyuki Kawano  
*The Journal of Physical Chemistry B* 2015 119 (1), 228-237

## **25. Exploring the Aqueous Vertical Ionization of Organic Molecules by Molecular Simulation and Liquid Microjet Photoelectron Spectroscopy**

Peter R. Tentscher, Robert Seidel, Bernd Winter, Jennifer J. Guerard, and J. Samuel Arey  
*The Journal of Physical Chemistry B* 2015 119 (1), 238-256

## **26. Diffusion–Viscosity Decoupling in Supercooled Glycerol Aqueous Solutions**

José A. Trejo González, M. Paula Longinotti, and Horacio R. Corti  
*The Journal of Physical Chemistry B* 2015 119 (1), 257-262

## **27. Effects of Water Concentration on the Free Volume of Amino Acid Ionic Liquids Investigated by Molecular Dynamics Simulations**

Abdul Rajjak Shaikh, Eiji Kamio, Hiromitsu Takaba, and Hideto Matsuyama  
*The Journal of Physical Chemistry B* 2015 119 (1), 263-273

## **28. Reorientational Jump Dynamics and Its Connections to Hydrogen Bond Relaxation in Molten Acetamide: An All-Atom Molecular Dynamics Simulation Study**

Suman Das, Ranjit Biswas, and Biswaroop Mukherjee  
*The Journal of Physical Chemistry B* 2015 119 (1), 274-283

## **29. Influence of Ultrasonic Frequency on Swan Band Sonoluminescence and Sonochemical Activity in Aqueous tert-Butyl Alcohol Solutions**

Rachel Pflieger, Abdoul Aziz Ndiaye, Tony Chave, and Sergey I. Nikitenko  
*The Journal of Physical Chemistry B* 2015 119 (1), 284-290

## **30. New Structural Anomaly Induced by Nanoconfinement**

Leandro B. Krott, José Rafael Bordin, and Marcia C. Barbosa  
*The Journal of Physical Chemistry B* 2015 119 (1), 291-300

## **31. Solvent-Dependent Enthalpic versus Entropic Anion Binding by Biaryl Substituted Quinoline Based Anion Receptors**

Zhan-Hu Sun, Markus Albrecht, Gerhard Raabe, Fang-Fang Pan, and Christoph Räuber  
*The Journal of Physical Chemistry B* 2015 119 (1), 301-306

## **32. Indolinoxazolidine: A Versatile Switchable Unit**

György Szalóki, Olivier Alévêque, Jean-Luc Pozzo, Rachid Hadji, Eric Levillain, and Lionel Sanguinet  
*The Journal of Physical Chemistry B* **2015** 119 (1), 307-315

### **33. Protein-Like Dynamics of Polycarbonate Polymers in Water**

Jernej Zidar, Geraldine S. Lim, Daniel W. Cheong, and Marco Klähn  
*The Journal of Physical Chemistry B* **2015** 119 (1), 316-329

### **34. Aggregation Behavior of Rod–Coil–Rod Triblock Copolymers in a Coil-Selective Solvent**

Ahmad K. Omar, Ben Hanson, Ryan T. Haws, Zhongjian Hu, David A. Vanden Bout, Peter J. Rossky, and Venkat Ganesan  
*The Journal of Physical Chemistry B* **2015** 119 (1), 330-337

### **35. Crystallization Behavior of Single Isotactic Poly(methyl methacrylate) Chains Visualized by Atomic Force Microscopy**

Takahiro Anzai, Mariko Kawauchi, Takehiro Kawauchi, and Jiro Kumaki  
*The Journal of Physical Chemistry B* **2015** 119 (1), 338-347

### **36. Surface Adsorption of Oppositely Charged C14TAB-PAMPS Mixtures at the Air/Water Interface and the Impact on Foam Film Stability**

Heiko Fauser, Regine von Klitzing, and Richard A. Campbell  
*The Journal of Physical Chemistry B* **2015** 119 (1), 348-358

### **37. Effects of Sodium Dodecyl Sulfate on Structures of Poly(N-isopropylacrylamide) at the Particle Surface**

Peng Wei Zhu  
*The Journal of Physical Chemistry B* **2015** 119 (1), 359-371

### **38. Hydrogen Bonds and Ionic Forms versus Polymerization of Imidazole at High Pressures**

Bharat Bhooshan Sharma, Ashok K. Verma, Susy Thomas, Chitra Murli, and Surinder M. Sharma  
*The Journal of Physical Chemistry B* **2015** 119 (1), 372-378

### **39. Correction to “Photophysics and Rotational Diffusion of Hydrophilic Molecule in Polymer and Polyols”**

Aninda Chatterjee, Banibrata Maity, Sayeed Ashique Ahmed, and Debabrata Seth  
*The Journal of Physical Chemistry B* **2015** 119 (1), 379-379