

APRIL 30, 2015

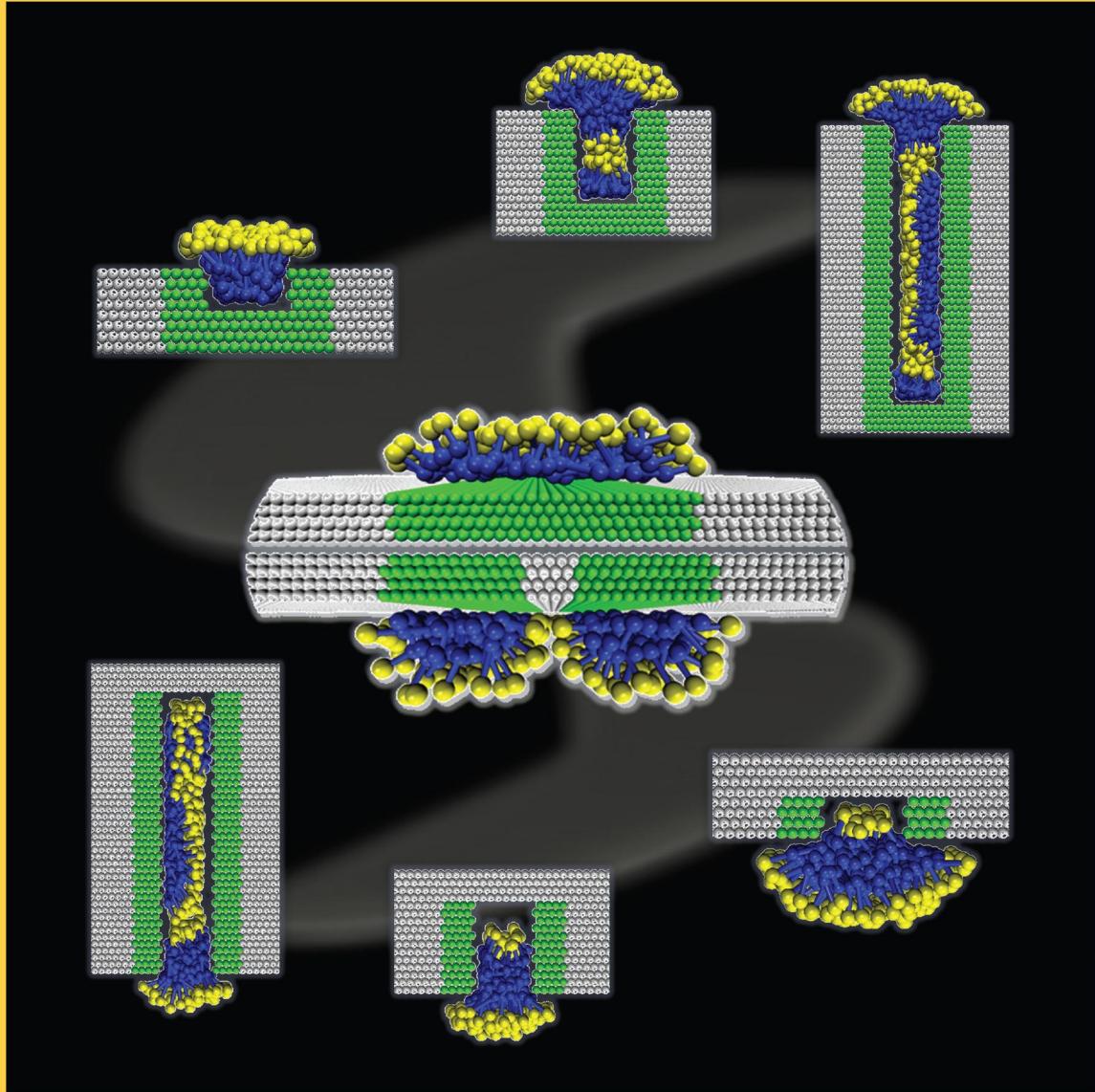
VOLUME 119

NUMBER 17

[pubs.acs.org/JPCB](http://pubs.acs.org/JPCB)THE JOURNAL OF  
PHYSICAL  
CHEMISTRY B

B

Morphological  
Transitions of  
Self-Assembled  
Aggregates in  
Chemically Patterned  
Trenches  
(see page 5467)



BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



ACS Publications  
Most Trusted. Most Cited. Most Read.

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

# THE JOURNAL OF PHYSICAL CHEMISTRY B

April 30, 2015: Vol. 119, Iss. 17

## Content

- 1. Pursuit-and-Evasion Reaction-Diffusion Waves in Microreactors with Tailored Geometry**  
A. Zambrano, A. S. Zadorin, Y. Rondelez, A. Estévez-Torres, and J.-C. Galas  
*The Journal of Physical Chemistry B* 2015 119 (17), 5349-5355  
DOI: 10.1021/jp509474w
- 2. Differential Interactions of Gelatin Nanoparticles with the Major Lipids of Model Lung Surfactant: Changes in the Lateral Membrane Organization**  
Weiam Daear, Patrick Lai, Max Anikovskiy, and Elmar J. Prenner  
*The Journal of Physical Chemistry B* 2015 119 (17), 5356-5366  
DOI: 10.1021/jp5122239
- 3. Dominant Alcohol–Protein Interaction via Hydration-Enabled Enthalpy-Driven Binding Mechanism**  
Yuan Chong, Alfred Kleinhammes, Pei Tang, Yan Xu, and Yue Wu  
*The Journal of Physical Chemistry B* 2015 119 (17), 5367-5375  
DOI: 10.1021/acs.jpcb.5b00378
- 4. NMR Analysis of Tuning Cross-Strand Phe/Tyr/Trp–Trp Interactions in Designed β-Hairpin Peptides: Terminal Switch from I to d Amino Acid as a Strategy for β-Hairpin Capping**  
Kamlesh M. Makwana and Radhakrishnan Mahalakshmi  
*The Journal of Physical Chemistry B* 2015 119 (17), 5376-5385  
DOI: 10.1021/acs.jpcb.5b00554
- 5. Redox Potentials of Protein Disulfide Bonds from Free-Energy Calculations**  
Wenjin Li, Ilona B. Baldus, and Frauke Gräter  
*The Journal of Physical Chemistry B* 2015 119 (17), 5386-5391  
DOI: 10.1021/acs.jpcb.5b01051
- 6. Theoretical Study on Reaction Mechanisms of Nitrite Reduction by Copper Nitrite Complexes: Toward Understanding and Controlling Possible Mechanisms of Copper Nitrite Reductase**  
Shintaro Maekawa, Toru Matsui, Kimihiko Hirao, and Yasuteru Shigeta  
*The Journal of Physical Chemistry B* 2015 119 (17), 5392-5403  
DOI: 10.1021/acs.jpcb.5b01356
- 7. Energy Thresholds of DNA Damage Induced by UV Radiation: An XPS Study**  
P. J. Gomes, A. M. Ferraria, A. M. Botelho do Rego, S. V. Hoffmann, P. A. Ribeiro, and M. Raposo  
*The Journal of Physical Chemistry B* 2015 119 (17), 5404-5411  
DOI: 10.1021/acs.jpcb.5b01439
- 8. Osmotic Compression of Anisotropic Proteins: Interaction Properties and Associated Structures in Wheat Gliadin Dispersions**  
Adeline Boire, Paul Menut, Marie-Hélène Morel, and Christian Sanchez  
*The Journal of Physical Chemistry B* 2015 119 (17), 5412-5421  
DOI: 10.1021/acs.jpcb.5b01673
- 9. Direct 765 nm Optical Excitation of Molecular Oxygen in Solution and in Single Mammalian Cells**  
Mikkel Bregnhøj, Alfonso Blázquez-Castro, Michael Westberg, Thomas Breitenbach, and Peter R. Ogilby

**10. Free Energy Surface of the Michaelis Complex of Lactate Dehydrogenase: A Network Analysis of Microsecond Simulations**

Xiaoliang Pan and Steven D. Schwartz

*The Journal of Physical Chemistry B* 2015 119 (17), 5430-5436

DOI: 10.1021/acs.jpcb.5b01840

**11. Random-Coil Behavior of Chemically Denatured Topologically Knotted Proteins Revealed by Small-Angle X-ray Scattering**

Po-Min Shih, Iren Wang, Yun-Tzai Cloud Lee, Shu-Ju Hsieh, Szu-Yu Chen, Liang-Wei Wang, Chih-Ting Huang, Chih-Ta Chien, Chia-Yun Chang, and Shang-Te Danny Hsu

*The Journal of Physical Chemistry B* 2015 119 (17), 5437-5443

DOI: 10.1021/acs.jpcb.5b01984

**12. A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins**

Bella L. Grigorenko, Alexander V. Nemukhin, Igor V. Polyakov, Maria G. Khrenova, and Anna I. Krylov

*The Journal of Physical Chemistry B* 2015 119 (17), 5444-5452

DOI: 10.1021/acs.jpcb.5b02271

**13. Adiabaticity of the Proton-Coupled Electron-Transfer Step in the Reduction of Superoxide Effected by Nickel-Containing Superoxide Dismutase Metallopeptide-Based Mimics**

Jason Shearer, Jennifer C. Schmitt, and Heather S. Clewett

*The Journal of Physical Chemistry B* 2015 119 (17), 5453-5461

DOI: 10.1021/acs.jpcb.5b02640

**14. Delocalized Hole Domains in Guanine-Rich DNA Oligonucleotides**

Amedeo Capobianco, Tonino Caruso, Anna Maria D'Ursi, Sandra Fusco, Annalisa Masi, Mario Scrima, Chrysostomos Chatgilialoglu, and Andrea Peluso

*The Journal of Physical Chemistry B* 2015 119 (17), 5462-5466

DOI: 10.1021/acs.jpcb.5b02940

**15. Surfactant Aggregates Tempered by Lateral Confinement**

Manaswee Suttipong, Brian P. Grady, and Alberto Striolo

*The Journal of Physical Chemistry B* 2015 119 (17), 5467-5474

DOI: 10.1021/jp511427m

**16. Probing the Effect of miRNA on siRNA-PEI Polyplexes**

Deniz Meneksedag-Erol, Tian Tang, and Hasan Uludağ

*The Journal of Physical Chemistry B* 2015 119 (17), 5475-5486

DOI: 10.1021/acs.jpcb.5b00415

**17. A Ring to Rule Them All: The Effect of Cyclopropane Fatty Acids on the Fluidity of Lipid Bilayers**

David Poger and Alan E. Mark

*The Journal of Physical Chemistry B* 2015 119 (17), 5487-5495

DOI: 10.1021/acs.jpcb.5b00958

**18. Density Functional Theory Study on the Cross-Linking of Mussel Adhesive Proteins**

Mohammad A. Matin, Ramesh Kumar Chitumalla, Manho Lim, Xingfa Gao, and Joonkyung Jang

*The Journal of Physical Chemistry B* 2015 119 (17), 5496-5504

DOI: 10.1021/acs.jpcb.5b01152

**19. Carboxylate Ion Pairing with Alkali-Metal Ions for  $\beta$ -Lactoglobulin and Its Role on Aggregation and Interfacial Adsorption**

Frank R. Beierlein, Timothy Clark, Björn Braunschweig, Kathrin Engelhardt, Lena Glas, and Wolfgang Peukert

*The Journal of Physical Chemistry B* 2015 119 (17), 5505-5517

DOI: 10.1021/acs.jpcb.5b01944

**20. Conformational Preadjustment in Aqueous Claisen Rearrangement Revealed by SITS-QM/MM MD Simulations**

Jun Zhang, Yi Isaac Yang, Lijiang Yang, and Yi Qin Gao  
*The Journal of Physical Chemistry B* 2015 119 (17), 5518-5530  
DOI: 10.1021/jp511057f

**21. Linkage Isomerization via Geminate Cage or Bimolecular Mechanisms: Time-Resolved Investigations of an Organometallic Photochrome**

Kristy M. DeWitt, Tung T. To, Edwin J. Heilweil, and Theodore J. Burkay  
*The Journal of Physical Chemistry B* 2015 119 (17), 5531-5536  
DOI: 10.1021/jp513033j

**22. Dissociation of Equimolar Mixtures of Aqueous Carboxylic Acids in Ionic Liquids: Role of Specific Interactions**

Shashi Kant Shukla and Anil Kumar  
*The Journal of Physical Chemistry B* 2015 119 (17), 5537-5545  
DOI: 10.1021/acs.jpcb.5b00056

**23. Water Effect on Acid-Gas Capture Using Choline Lactate: A DFT Insight beyond Molecule-Molecule Pair Simulations**

Gregorio García, Mert Atilhan, and Santiago Aparicio  
*The Journal of Physical Chemistry B* 2015 119 (17), 5546-5557  
DOI: 10.1021/acs.jpcb.5b00184

**24. Hygroscopicity of Mixed Glycerol/Mg(No<sub>3</sub>)<sub>2</sub>/Water Droplets Affected by the Interaction between Magnesium Ions and Glycerol Molecules**

Yang Wang, Jia-Bi Ma, Qiang Zhou, Shu-Feng Pang, and Yun-Hong Zhang  
*The Journal of Physical Chemistry B* 2015 119 (17), 5558-5566  
DOI: 10.1021/acs.jpcb.5b00458

**25. Surface Tension of Supercooled Water Determined by Using a Counterpressure Capillary Rise Method**

Václav Vinš, Maurice Fransen, Jiří Hykl, and Jan Hrubý  
*The Journal of Physical Chemistry B* 2015 119 (17), 5567-5575  
DOI: 10.1021/acs.jpcb.5b00545

**26. Hydration and Hydrogen Bond Network of Water during the Coil-to-Globule Transition in Poly(N-isopropylacrylamide) Aqueous Solution at Cloud Point Temperature**

Keiichiro Shiraga, Hirotaka Naito, Tetsuhito Suzuki, Naoshi Kondo, and Yuichi Ogawa  
*The Journal of Physical Chemistry B* 2015 119 (17), 5576-5587  
DOI: 10.1021/acs.jpcb.5b01021

**27. Octanol-Water Partition Coefficient from 3D-RISM-KH Molecular Theory of Solvation with Partial Molar Volume Correction**

WenJuan Huang, Nikolay Blinov, and Andriy Kovalenko  
*The Journal of Physical Chemistry B* 2015 119 (17), 5588-5597  
DOI: 10.1021/acs.jpcb.5b01291

**28. Gibbs Excess and the Calculation of the Absolute Surface Composition of Liquid Binary Mixtures**

Carolina Bermúdez-Salguero and Jesús Gracia-Fadrique  
*The Journal of Physical Chemistry B* 2015 119 (17), 5598-5608  
DOI: 10.1021/acs.jpcb.5b01436

**29. Accurate Measurements of Dielectric and Optical Functions of Liquid Water and Liquid Benzene in the VUV Region (1–100 eV) Using Small-Angle Inelastic X-ray Scattering**

Hisashi Hayashi and Nozomu Hiraoka  
*The Journal of Physical Chemistry B* 2015 119 (17), 5609-5623  
DOI: 10.1021/acs.jpcb.5b01567

**30. Thermodynamic Profiles of Salt Effects on a Host–Guest System: New Insight into the Hofmeister Effect**

Corinne L. D. Gibb, Estelle E. Oertling, Santhosh Velaga, and Bruce C. Gibb  
*The Journal of Physical Chemistry B* 2015 119 (17), 5624-5638

DOI: 10.1021/acs.jpcb.5b01708

### 31. Programmable DNA-Mediated Multitasking Processor

Jian-Jun Shu, Qi-Wen Wang, Kian-Yan Yong, Fangwei Shao, and Kee Jin Lee  
*The Journal of Physical Chemistry B* 2015 119 (17), 5639-5644  
DOI: 10.1021/acs.jpcb.5b02165

### 32. Configurational Entropy in Thermoset Polymers

Martin Jensen and Johnny Jakobsen  
*The Journal of Physical Chemistry B* 2015 119 (17), 5645-5649  
DOI: 10.1021/jp510836y

### 33. Proton Transfer Dynamics of 4'-N,N-Dimethylamino-3-hydroxyflavone Observed in Hydrogen-Bonding Solvents and Aqueous Micelles

Deborin Ghosh, Shaikh Batuta, Sreeparna Das, Naznin Ara Begum, and Debabrata Mandal  
*The Journal of Physical Chemistry B* 2015 119 (17), 5650-5661  
DOI: 10.1021/acs.jpcb.5b00021

### 34. Topographic Characterization of Cu–Ni NPs @ a-C:H Films by AFM and Multifractal Analysis

Ştefan Tălu, Sebastian Stach, Tayebeh Ghodselahti, Atefeh Ghaderi, Shahram Solaymani, Arash Boochani, and Żaneta Garczyk  
*The Journal of Physical Chemistry B* 2015 119 (17), 5662-5670  
DOI: 10.1021/acs.jpcb.5b00042

### 35. Isotropic–Nematic Phase Transition in Hard Platelets as Described by a Third-Virial Theory

Giorgio Cinacchi and Alessandro Tani  
*The Journal of Physical Chemistry B* 2015 119 (17), 5671-5676  
DOI: 10.1021/acs.jpcb.5b00389

### 36. Reconsidering the Dynamics in Mixtures of Methyltetrahydrofuran with Tristrene and Polystyrene

K. L. Ngai and S. Capaccioli  
*The Journal of Physical Chemistry B* 2015 119 (17), 5677-5684  
DOI: 10.1021/acs.jpcb.5b00488

### 37. Enhanced Charge-Transfer Emission in Polyimides by Cyano-Groups Doping

María San Sebastián, Virginia Martínez-Martínez, Alberto Maceiras, José Luis Vilas, Iñigo López-Arbeloa, and Luis Manuel León  
*The Journal of Physical Chemistry B* 2015 119 (17), 5685-5692  
DOI: 10.1021/acs.jpcb.5b00845

### 38. Mass and Charge Transport in the Polymer–Ionic-Liquid System PEO-EMImI: From Ionic-Liquid-in-Polymer to Polymer-in-Ionic-Liquid Electrolytes

Johannes Kösters, Monika Schönhoff, and Nicolaas A. Stolwijk  
*The Journal of Physical Chemistry B* 2015 119 (17), 5693-5700  
DOI: 10.1021/acs.jpcb.5b01113

### 39. Na/Ca Intermixing around Silicate and Phosphate Groups in Bioactive Phosphosilicate Glasses Revealed by Heteronuclear Solid-State NMR and Molecular Dynamics Simulations

Renny Mathew, Baltzar Stevensson, and Mattias Edén  
*The Journal of Physical Chemistry B* 2015 119 (17), 5701-5715  
DOI: 10.1021/acs.jpcb.5b01130

### 40. Shear-Induced Precursor Relaxation-Dependent Growth Dynamics and Lamellar Orientation of $\beta$ -Crystals in $\beta$ -Nucleated Isotactic Polypropylene

Yan-Hui Chen, Du-Fei Fang, Jun Lei, Liang-Bin Li, Benjamin S. Hsiao, and Zhong-Ming Li  
*The Journal of Physical Chemistry B* 2015 119 (17), 5716-5727  
DOI: 10.1021/acs.jpcb.5b01480

**41. N-Heterocyclic Carbene-Catalyzed Ring Opening Polymerization of  $\epsilon$ -Caprolactone with and without Alcohol Initiators: Insights from Theory and Experiment**

Gavin O. Jones, Young A. Chang, Hans W. Horn, Ashwin K. Acharya, Julia E. Rice, James L. Hedrick, and Robert M. Waymouth  
*The Journal of Physical Chemistry B* 2015 119 (17), 5728-5737  
DOI: 10.1021/acs.jpcb.5b01595

**42. Supramolecular Polymerization: A Coarse Grained Molecular Dynamics Study**

Karteek K. Bejagam and Sundaram Balasubramanian  
*The Journal of Physical Chemistry B* 2015 119 (17), 5738-5746  
DOI: 10.1021/acs.jpcb.5b01655

**43.  $^{77}\text{Se}$  Nuclear Spin–Lattice Relaxation in Binary Ge–Se Glasses: Insights into Floppy Versus Rigid Behavior of Structural Units**

Sabyasachi Sen, Derrick C. Kaseman, Ivan Hung, and Zhehong Gan  
*The Journal of Physical Chemistry B* 2015 119 (17), 5747-5753  
DOI: 10.1021/acs.jpcb.5b01934