

APRIL 3, 2014

VOLUME 118

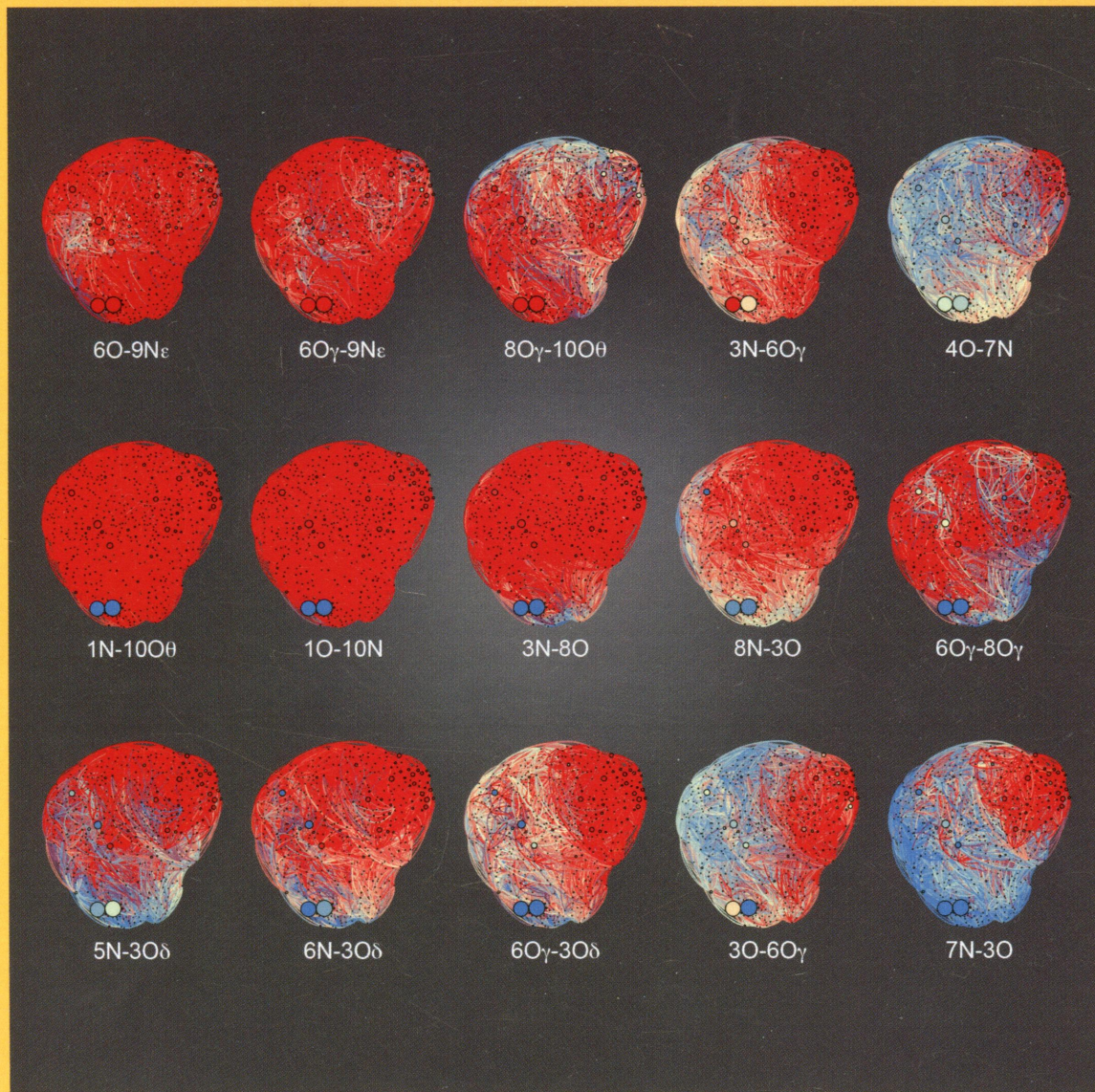
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# THE JOURNAL OF PHYSICAL CHEMISTRY

B

Configuration Space  
Networks of Chignolin  
Reveal How  
Hydrogen Bonds  
Guide Folding  
(see page 5A)



BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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**ON THE COVER:** Configuration space networks of chignolin reveal how hydrogen bonds guide folding. In Dickson et al., an algorithm ("WExplore") is introduced that enhances sampling and allows for the efficient construction of configuration space networks. In CSNs, each node (circle) represents a configuration of the system, and the edges (lines) join together configurations that are connected by transitions during sampling. The native state is composed of the two large nodes at the bottom left, and the top right states are the most unfolded. The nodes on the cover are colored according to the distance between various native and nonnative hydrogen bonding pairs, with blue indicating the pairs are within hydrogen-bonding distance, and red indicating they are far away. This visualization technique allows for the easy identification of nonnative interactions that help guide folding (such as 4O–7N) as well as native hydrogen bonds that are formed early (7N–3O) or late (1O–10N) in the folding process. See page 3532.

## Articles

### Biophysical Chemistry and Biomolecules

- 3479  [dx.doi.org/10.1021/jp4106037](https://doi.org/10.1021/jp4106037)  
**Oxidation and Nitration of Tyrosine by Ozone and Nitrogen Dioxide: Reaction Mechanisms and Biological and Atmospheric Implications**  
L. Sandhiya, P. Kolandaivel, and K. Senthikumar\*
- 3491  [dx.doi.org/10.1021/jp409543p](https://doi.org/10.1021/jp409543p)  
**Investigating Water Interactions with Collagen Using  $^2\text{H}$  Multiple Quantum Filtered NMR Spectroscopy To Provide Insights into the Source of Double Quantum Filtered Signal in Tissue**  
Cassidy R. VanderSchee and Kristopher J. Ooms\*
- 3498 [dx.doi.org/10.1021/jp4097327](https://doi.org/10.1021/jp4097327)  
**Evidence for Two New Solution States of Ubiquitin by IMS–MS Analysis**  
Huilin Shi and David E. Clemmer\*
- 3507 [dx.doi.org/10.1021/jp410477x](https://doi.org/10.1021/jp410477x)  
**Free Energy of Lipid Bilayer Defects Affected by Alzheimer's Disease-Associated Amyloid- $\beta_{42}$  Monomers**  
Tobias Pobandt and Volker Knecht\*
- 3517  [dx.doi.org/10.1021/jp411122h](https://doi.org/10.1021/jp411122h)  
**The Stability of a  $\beta$ -Hairpin Is Altered by Surface–Water Interactions under Confinement**  
J. Srinivasa Rao, Micholas Dean Smith, and Luis Cruz\*

3524  [dx.doi.org/10.1021/jp411174t](https://doi.org/10.1021/jp411174t)

**2D Spectroscopy Study of Water-Soluble Chlorophyll-Binding Protein from *Lepidium virginicum***

Jan Alster, Heiko Lokstein, Jakub Dostál, Akira Uchida, and Donatas Zigmantas\*

3532 [dx.doi.org/10.1021/jp411479c](https://doi.org/10.1021/jp411479c)

**WExplore: Hierarchical Exploration of High-Dimensional Spaces Using the Weighted Ensemble Algorithm**

Alex Dickson and Charles L. Brooks III\*

3543  [dx.doi.org/10.1021/jp4125099](https://doi.org/10.1021/jp4125099)


**Evaluation of Enhanced Sampling Provided by Accelerated Molecular Dynamics with Hamiltonian Replica Exchange Methods**

Daniel R. Roe, Christina Bergonzo, and Thomas E. Cheatham III\*

3553  [dx.doi.org/10.1021/jp500362q](https://doi.org/10.1021/jp500362q)

**Ab Initio Modeling of the Effect of Oxidation Coupled with H<sub>2</sub>O Deprotonation on Carboxylate Ligands in Mn/Ca Clusters**

Wooi Yee Chuah, Rob Stranger,\* Ron J. Pace,\* Elmars Krausz,\* and Terry J. Frankcombe\*

3559  [dx.doi.org/10.1021/jp501114h](https://doi.org/10.1021/jp501114h)

**$\alpha$ -Synuclein's Adsorption, Conformation, and Orientation on Cationic Gold Nanoparticle Surfaces Seeds Global Conformation Change**

Jie An Yang, Wayne Lin, Wendy S. Woods, Julia M. George, and Catherine J. Murphy\*

3572  [dx.doi.org/10.1021/jp501622d](https://doi.org/10.1021/jp501622d)

**How To Tackle the Issues in Free Energy Simulations of Long Amphiphiles Interacting with Lipid Membranes: Convergence and Local Membrane Deformations**

Hugo A. L. Filipe, Maria João Moreno, Tomasz Róg, Ilpo Vattulainen,\* and Luís M. S. Loura\*

## **Biomaterials, Surfactants, and Membranes**

3582  [dx.doi.org/10.1021/jp4069703](https://doi.org/10.1021/jp4069703)

**Effect of Hydroxyl Group Substituted Spacer Group of Cationic Gemini Surfactants on Solvation Dynamics and Rotational Relaxation of Coumarin-480 in Aqueous Micelles**

Amit K. Tiwari, Sonu, and Subit K. Saha\*

3593 [dx.doi.org/10.1021/jp410636w](https://doi.org/10.1021/jp410636w)

**Solubilization in Mixed Micelles Studied by Molecular Dynamics Simulations and COSMOmic**

Sandra Storm,\* Sven Jakobtorweihen, and Irina Smirnova

3605 [dx.doi.org/10.1021/jp410882r](https://doi.org/10.1021/jp410882r)

**Phase Separation in Phosphatidylcholine Membrane Caused by the Presence of a Pyrimidine Analogue of Fluphenazine with High Anti-Multidrug-Resistance Activity**

Katarzyna Cieřlik-Boczula,\* Piotr Świątek, Agata Jaszczyszyn, Patrycja Zawilska, Kazimierz Gąsiorowski, Wiesław Malinka, and Gottfried Köhler

3616  [dx.doi.org/10.1021/jp411648s](https://doi.org/10.1021/jp411648s)

**AH Peptide-Mediated Formation of Charged Planar Lipid Bilayers**

Goh Haw Zan, Joshua A. Jackman, and Nam-Joon Cho\*

3622 [dx.doi.org/10.1021/jp5009797](https://doi.org/10.1021/jp5009797)

**Dynamic Phase Diagram of a Nonionic Surfactant Lamellar Phase**

Luigi Gentile,\* Manja A. Behrens, Sandor Balog, Kell Mortensen, Giuseppe A. Ranieri, and Ulf Olsson

## Liquids; Chemical and Dynamical Processes in Solution

3630 [dx.doi.org/10.1021/jp4072229](https://doi.org/10.1021/jp4072229)

**Stability Analysis of Microdrops during Concentrating Processes**

Fatemeh Eslami and Janet A. W. Elliott\*

3642  [dx.doi.org/10.1021/jp410168t](https://doi.org/10.1021/jp410168t)

**Effect of Side-Chain Length on Structural and Dynamic Properties of Ionic Liquids with Hydroxyl Cationic Tails**

Kuo Wei, Li Deng, Yanting Wang,\* Zhong-Can Ou-Yang, and Guodong Wang

3650 [dx.doi.org/10.1021/jp410260g](https://doi.org/10.1021/jp410260g)

**Understanding the Role of the Cosolvent in the Zeolite Template Function of Imidazolium-Based Ionic Liquid**

Regla Ayala,\* Svetlana Ivanova, José Maria Martínez Blanes, Francisca Romero-Sarria, and José Antonio Odriozola

3661 [dx.doi.org/10.1021/jp411765f](https://doi.org/10.1021/jp411765f)

**Wetting and Tribological Properties of Ionic Liquids**

Henry J. Castejón,\* Troy J. Wynn, and Zachary M. Marcin

3669 [dx.doi.org/10.1021/jp411778q](https://doi.org/10.1021/jp411778q)

**Exploring the Photophysics of Curcumin in Zwitterionic Micellar System: An Approach to Control ESIPT Process in the Presence of Room Temperature Ionic Liquids (RTILs) and Anionic Surfactant**

Chiranjib Banerjee, Surajit Ghosh, Sarthak Mandal, Jagannath Kuchlyan, Niloy Kundu, and Nilmoni Sarkar\*

3682  [dx.doi.org/10.1021/jp500790r](https://doi.org/10.1021/jp500790r)

**One of the Distinctive Properties of Ionic Liquids over Molecular Solvents and Inorganic Salts: Enhanced Basicity Stemming from the Electrostatic Environment and "Free" Microstructure**

Qiwei Yang, Huabin Xing,\* Zongbi Bao, Baogen Su, Zhiguo Zhang, Yiwen Yang, Sheng Dai, and Qilong Ren\*

3689  [dx.doi.org/10.1021/jp500877u](https://doi.org/10.1021/jp500877u)  
**Coordination Number of  $\text{Li}^+$  in Nonaqueous Electrolyte Solutions Determined by Molecular Rotational Measurements**  
Kaijun Yuan, Hongtao Bian, Yuneng Shen, Bo Jiang, Jiebo Li, Yufan Zhang, Hailong Chen, and Junrong Zheng\*

3696  [dx.doi.org/10.1021/jp5009994](https://doi.org/10.1021/jp5009994)  
**Regional Electrophilic and Nucleophilic Fukui Functions Efficiently Highlight the Lewis Acidic/Basic Regions in Ionic Liquids**  
Andrea Cerda-Monje,\* Rodrigo Ormazábal-Toledo,\* Carlos Cárdenas, Patricio Fuentealba, and Renato Contreras

3702 [dx.doi.org/10.1021/jp501344t](https://doi.org/10.1021/jp501344t)  
**Changes in Permittivity and Density of Molecular Liquids under High Pressure**  
Vladimir D. Kiselev,\* Dmitry A. Kornilov, and Alexander I. Kononov

## Glasses, Colloids, Polymers, and Soft Matter

3710 [dx.doi.org/10.1021/jp411942t](https://doi.org/10.1021/jp411942t)  
**Short Range Structural Models of the Glass Transition Temperatures and Densities of  $0.5\text{Na}_2\text{S} + 0.5[x\text{GeS}_2 + (1 - x)\text{PS}_{5/2}]$  Mixed Glass Former Glasses**  
Christian Bischoff, Katherine Schuller, and Steve W. Martin\*

3720 [dx.doi.org/10.1021/jp4121782](https://doi.org/10.1021/jp4121782)  
**Characteristics of the Structural and Johari–Goldstein Relaxations in Pd-Based Metallic Glass-Forming Liquids**  
Jichao Qiao, Riccardo Casalini, Jean-Marc Pelletier,\* and Hidemi Kato

3731 [dx.doi.org/10.1021/jp412440g](https://doi.org/10.1021/jp412440g)  
**Molecular Dynamics of Spherical Nanoparticles in Dense Polymer Melts**  
Alessandro Patti\*

3743  [dx.doi.org/10.1021/jp4127978](https://doi.org/10.1021/jp4127978)  
**Phase Structure and Phase Transition Mechanism for Light-Induced *1a3d* Cubic Phase in 4'-*n*-Docosyloxy-3'-nitrobiphenyl-4-carboxylic acid/Ethyl 4-(4'-*n*-docosyloxyphenylazo)benzoate Binary Mixture**  
Ryo Hori, Yohei Miwa,\* Katsuhiko Yamamoto, and Shoichi Kutsumizu\*

3750 [dx.doi.org/10.1021/jp501325x](https://doi.org/10.1021/jp501325x)  
**Dynamics of Linear Poly(*N*-isopropylacrylamide) in Water around the Phase Transition Investigated by Dielectric Relaxation Spectroscopy**  
Marieke Füllbrandt, Elena Ermilova, Asad Asadujaman, Ralph Hölzel, Frank F. Bier, Regine von Klitzing, and Andreas Schönhals\*