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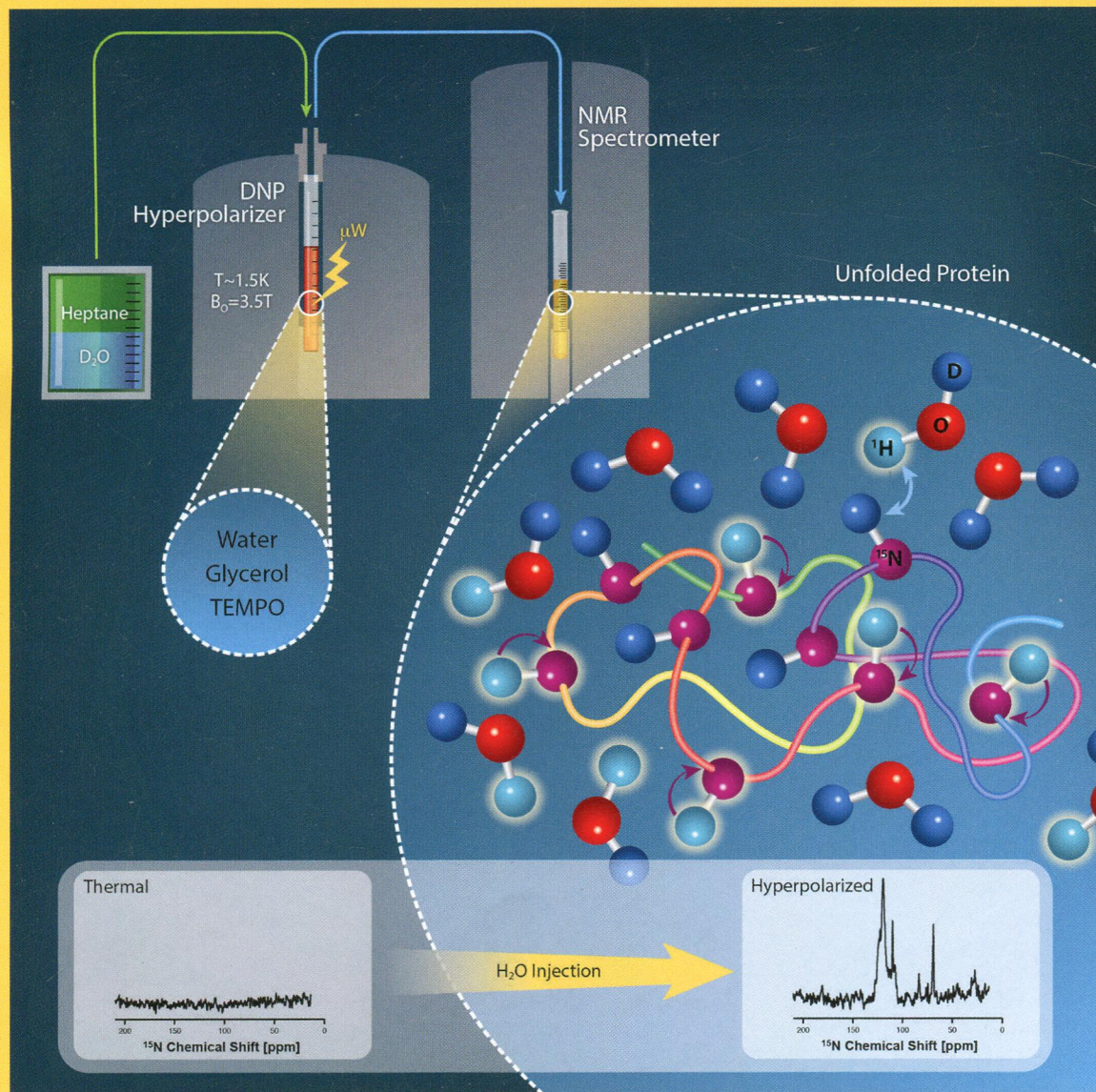
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# THE JOURNAL OF PHYSICAL CHEMISTRY

# B

Enhancing the  
Sensitivity of  
Solution-Phase  
Protein NMR by  
Optimized Injections of  
Hyperpolarized Water  
(see page 5A)



BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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**ON THE COVER:** Enhancing the sensitivity of solution-phase protein NMR by optimized injections of hyperpolarized water. A main obstacle arising when using *ex situ* hyperpolarization to increase the sensitivity of biomolecular NMR is the fast relaxation that spins undergo upon being transferred from the cryogenic polarizer to the room temperature spectrometer. To cope with this limitation, this study explores the use of hyperpolarized water: methods to achieve optimal spin polarization of H<sub>2</sub>O's protons were devised, and substantial spontaneous enhancement of certain <sup>1</sup>H and <sup>15</sup>N biomolecular resonances was observed upon using such hyperpolarized water to dissolve amino acids and polypeptides. See page 3281.

## Articles

### Biophysical Chemistry and Biomolecules

- 3245  [dx.doi.org/10.1021/jp4076299](https://doi.org/10.1021/jp4076299)  
**A DFT Study of the *cis*-Dihydroxylation of Nitroaromatic Compounds Catalyzed by Nitrobenzene Dioxigenase**  
 Anna Pabis, Inacrist Geronimo, and Piotr Paneth\*
- 
- 3257 [dx.doi.org/10.1021/jp409195c](https://doi.org/10.1021/jp409195c)  
**Aqueous Poly(amidoamine) Dendrimer G3 and G4 Generations with Several Interior Cores at pHs 5 and 7: A Molecular Dynamics Simulation Study**  
 Sajjad Kavyani, Sepideh Amjad-Iranagh, and Hamid Modarress\*
- 
- 3267  [dx.doi.org/10.1021/jp409201v](https://doi.org/10.1021/jp409201v)  
**New Solvates of an Old Drug Compound (Phenobarbital): Structure and Stability**  
 Neslihan Zencirci, Ulrich J. Griesser,\* Thomas Gelbrich, Volker Kahlenberg, Ram K. R. Jetti, David C. Apperley, and Robin K. Harris
- 
- 3281  [dx.doi.org/10.1021/jp4102916](https://doi.org/10.1021/jp4102916)  
**On the Potential of Hyperpolarized Water in Biomolecular NMR Studies**  
 Talia Harris, Or Szekely, and Lucio Frydman\*
- 
- 3291  [dx.doi.org/10.1021/jp4121222](https://doi.org/10.1021/jp4121222)  
**Ultrafast Dynamical Study of Pyrene-*N,N*-dimethylaniline (PyDMA) as an Organic Molecular Diode in Solid State**  
 Sreevidya Thekku Veedu,\* Dirk Raiser, Reza Kia, Mirko Scholz, and Simone Techert\*
- 
- 3298  [dx.doi.org/10.1021/jp500379e](https://doi.org/10.1021/jp500379e)  
**Fine Refinement of Solid-State Molecular Structures of Leu- and Met-Enkephalins by NMR Crystallography**  
 Tomasz Pawlak\* and Marek J. Potrzebowski\*

3310

[dx.doi.org/10.1021/jp500530h](https://doi.org/10.1021/jp500530h)**Solvent Effects on the Dynamics of Amyloidogenic Insulin Revealed by Neutron Spin Echo Spectroscopy**

Mirko Erkkamp, Sebastian Grobelny, Antonio Faraone, Claus Czeslik,\* and Roland Winter

3317

[dx.doi.org/10.1021/jp500774q](https://doi.org/10.1021/jp500774q)**How Quickly Can a  $\beta$ -Hairpin Fold from Its Transition State?**

Beatrice N. Markiewicz, Lijiang Yang, Robert M. Culik, Yi Qin Gao,\* and Feng Gai\*

3326

[dx.doi.org/10.1021/jp501890p](https://doi.org/10.1021/jp501890p)**Capping Amyloid  $\beta$ -Sheets of the Tau-Amyloid Structure VQIVYK with Hexapeptides Designed To Arrest Growth. An ONIOM and Density Functional Theory Study**

Joshua A. Plumley, Jorge Ali-Torres, Gabor Pohl, and J. J. Dannenberg\*

**Biomaterials, Surfactants, and Membranes**

3335

[dx.doi.org/10.1021/jp410401z](https://doi.org/10.1021/jp410401z)**The Structure of Lipid Bilayers Adsorbed on Activated Carboxy-Terminated Monolayers Investigated by Sum Frequency Generation Spectroscopy**

Michael T. L. Casford, Aimin Ge, Peter J. N. Kett, Shen Ye,\* and Paul B. Davies\*

3346

[dx.doi.org/10.1021/jp410612k](https://doi.org/10.1021/jp410612k)**Molecular Simulation of Protein Encapsulation in Vesicle Formation**

Bram van Hoof, Albert J. Markvoort,\* Rutger A. van Santen, and Peter A. J. Hilbers

3355

[dx.doi.org/10.1021/jp411618h](https://doi.org/10.1021/jp411618h)**Dynamic Behavior of the Active and Inactive States of the Adenosine A<sub>2A</sub> Receptor**

Sangbae Lee, Supriyo Bhattacharya, Reinhard Grisshammer, Christopher Tate, and Nagarajan Vaidehi\*

3366

[dx.doi.org/10.1021/jp411798s](https://doi.org/10.1021/jp411798s)**Toward Vibrational Dynamics at Liquid–Liquid and Nano-Interfaces: Time-Resolved Sum-Frequency Scattering**

Rüdiger Scheu and Sylvie Roke\*

**Liquids; Chemical and Dynamical Processes in Solution**

3372

[dx.doi.org/10.1021/jp4100729](https://doi.org/10.1021/jp4100729)**Colloidal Crystal Formation at the "Nafion–Water" Interface**

Nikolay F. Bunkin,\* Vladimir S. Gorelik, Valeriy A. Kozlov, Alexey V. Shkirin, and Nikolay V. Suyazov

3378

[dx.doi.org/10.1021/jp4116639](https://doi.org/10.1021/jp4116639)**Solvent Polarity Considerations Are Unable to Describe Fullerene Solvation Behavior**

Vitaly V. Chaban, Cleiton Maciel, and Eudes Eterno Fileti\*

3385 dx.doi.org/10.1021/jp411781n  
**Thermal Conductivity of Molten Alkali Metal Fluorides (LiF, NaF, KF) and Their Mixtures**  
Yoshiki Ishii, Keisuke Sato, Mathieu Salanne, Paul A. Madden, and Norikazu Ohtori\*

3392 dx.doi.org/10.1021/jp412260a  
**Can an Ab Initio Three-Body Virial Equation Describe the Mercury Gas Phase?**  
J. Wiebke,\* M. Wormit, R. Hellmann, E. Pahl, and P. Schwerdtfeger\*

3401 dx.doi.org/10.1021/jp500210n  
**Effect of Confinement on Excited-State Proton Transfer of Firefly's Chromophore *o*-Luciferin in AOT Reverse Micelles**  
Jagannath Kuchlyan, Debasis Banik, Niloy Kundu, Surajit Ghosh, Chiranjib Banerjee, and Nilmoni Sarkar\*

3409 dx.doi.org/10.1021/jp500296x  
**Quantitative Prediction of Physical Properties of Imidazolium Based Room Temperature Ionic Liquids through Determination of Condensed Phase Site Charges: A Refined Force Field**  
Anirban Mondal and Sundaram Balasubramanian\*

3423 dx.doi.org/10.1021/jp500817s  
**Molecular Dynamics Simulation Study of Methanesulfonic Acid**  
Manel Canales\* and Carlos Alemán

## Glasses, Colloids, Polymers, and Soft Matter

3431 dx.doi.org/10.1021/jp411616b  
**Blind Prediction of Binding Affinities for Charged Supramolecular Host–Guest Systems: Achievements and Shortcomings of DFT-D3**  
Rebecca Sure, Jens Antony, and Stefan Grimme\*

3441 dx.doi.org/10.1021/jp411888p  
**Terminal Index: A New Way for Precise Description of Topologic Structure of Highly Branched Polymers Derived from  $A_2 + B_3$  Stepwise Polymerization**  
Heng Chen and Jie Kong\*

3451 dx.doi.org/10.1021/jp412126n  
**Isothermal Behavior of the Soret Effect in Nonionic Microemulsions: Size Variation by Using Different *n*-Alkanes**  
Philipp Naumann, Sascha Datta, Thomas Sottmann,\* Bastian Art, Henrich Frielinghaus, and Simone Wiegand\*

3461 dx.doi.org/10.1021/jp4125233  
**Chain-Length-Dependent Autocatalytic Hydrolysis of Fatty Acid Anhydrides in Polyethylene Glycol**  
Cao Cao, Qing-Biao Wang, Lin-Jun Tang, Bing-Qiang Ge, Zhong-Xiu Chen,\* and Shao-Ping Deng

**Orientational Order of Two Fluoro- and Isothiocyanate-Substituted Nematogens by Combination of  $^{13}\text{C}$  NMR Spectroscopy and DFT Calculations**

Lucia Calucci,\* Elisa Carignani, Marco Geppi,\* Sara Macchi, Benedetta Mennucci, and Stanislaw Urban