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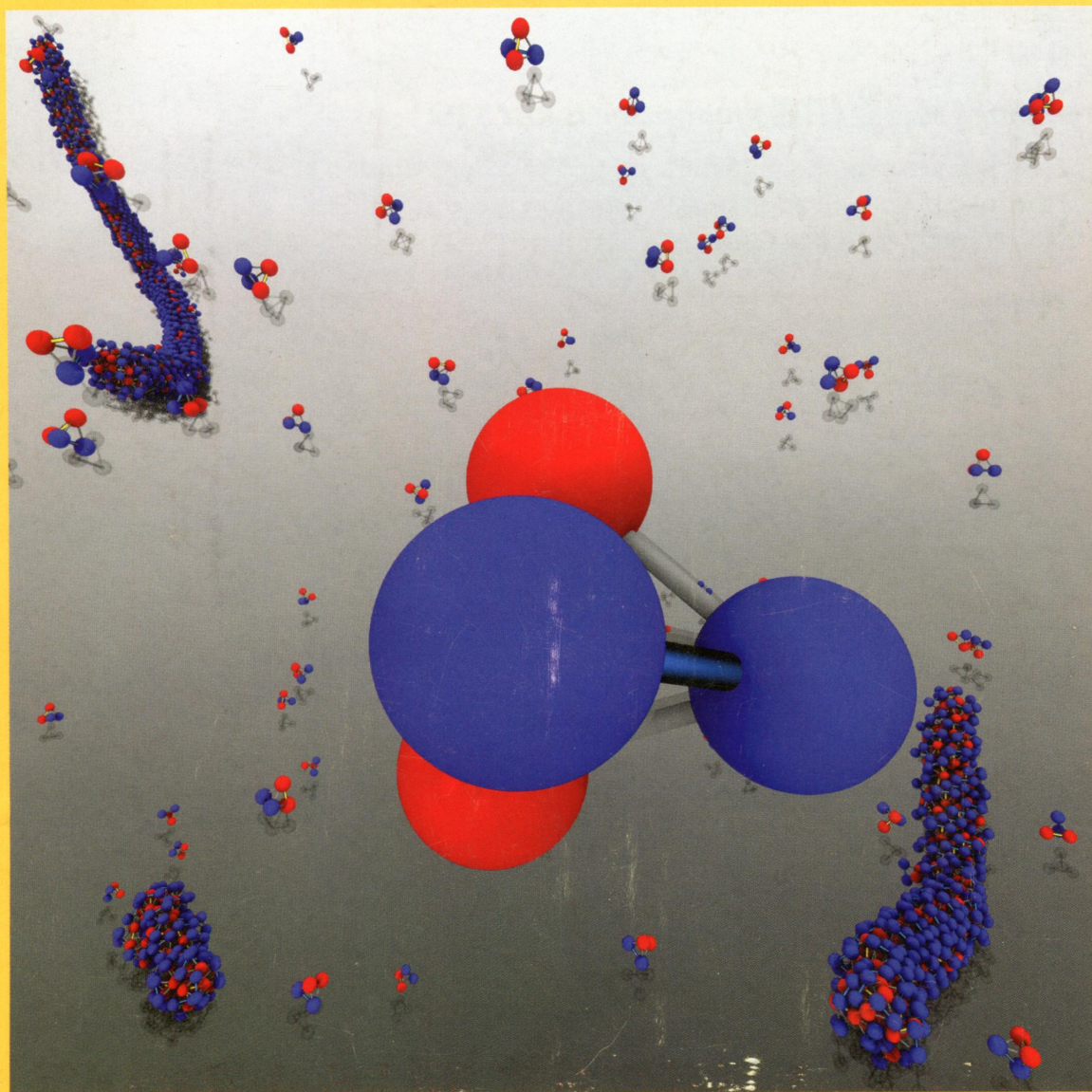
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# THE JOURNAL OF PHYSICAL CHEMISTRY

# B



Self-Assembly of  
Tetrahedron Molecules  
Comprising Two  
Attractive and Two  
Repulsive Beads  
(see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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**ON THE COVER:** Self-assembly of tetrahedron molecules comprising two attractive and two repulsive beads. A minimal self-assembly model with two attractive (red) and two repulsive (blue) beads bound into a tetrahedron captures an unexpected diversity and complexity of assembly pathways and structures. Self-assembly proceeds through formation of small quasi-spherical assemblies into large, elongated aggregates, which structurally convert into more ordered polymorphic aggregates, resembling the amyloid fibril morphology.

## Articles

### Biophysical Chemistry and Biomolecules

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[dx.doi.org/10.1021/jp412819j](https://doi.org/10.1021/jp412819j)

**Minimal Model of Self-Assembly: Emergence of Diversity and Complexity**  
Bogdan Barz and Brigita Urbanc\*

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[dx.doi.org/10.1021/jp409764z](https://doi.org/10.1021/jp409764z)

**Structural and Thermodynamic Studies on the Interaction of Iminium and Alkanolamine Forms of Sanguinarine with Hemoglobin**

Soumitra Hazra and Gopinatha Suresh Kumar\*

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[dx.doi.org/10.1021/jp411096d](https://doi.org/10.1021/jp411096d)

**Melting of DNA Nonoriented Fibers: A Wide-Angle X-ray Diffraction Study**

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[dx.doi.org/10.1021/jp4111234](https://doi.org/10.1021/jp4111234)

**Update to the General Amber Force Field for Small Solutes with an Emphasis on Free Energies of Hydration**

Joakim P. M. Jämbeck and Alexander P. Lyubartsev\*

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[dx.doi.org/10.1021/jp411136w](https://doi.org/10.1021/jp411136w)

**Sensitivity of Water Dynamics to Biologically Significant Surfaces of Monomeric Insulin: Role of Topology and Electrostatic Interactions**

Kushal Bagchi and Susmita Roy\*

3814  [dx.doi.org/10.1021/jp411387p](https://doi.org/10.1021/jp411387p)

**Molecular Organization of Crystalline  $\beta$ -Carotene in Carrots Determined with Polarization-Dependent Second and Third Harmonic Generation Microscopy**

Danielle Tokarz, Richard Cisek, Serguei Krouglov, Lukas Kontenis, Ulrich Fekl, and Virginijus Barzda\*

3823  [dx.doi.org/10.1021/jp412125d](https://doi.org/10.1021/jp412125d)

**Multiple Scale Dynamics in Proteins Probed at Multiple Time Scales through Fluctuations of NMR Chemical Shifts**

Paolo Calligaris\* and Daniel Abergel\*

3832  [dx.doi.org/10.1021/jp500404u](https://doi.org/10.1021/jp500404u)

**Exploring the Interaction of Bisphenol-S with Serum Albumins: A Better or Worse Alternative for Bisphenol A?**

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3844  [dx.doi.org/10.1021/jp500780m](https://doi.org/10.1021/jp500780m)

**Collision Dynamics of Protonated *N*-Acetylmethionine with Singlet Molecular Oxygen ( $a^1\Delta_g$ ): The Influence of the Amide Bond and Ruling Out the Complex-Mediated Mechanism at Low Energies**

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3853  [dx.doi.org/10.1021/jp501893c](https://doi.org/10.1021/jp501893c)

**Single-Molecule Fluorescence Resonance Energy Transfer Studies of the Human Telomerase RNA Pseudoknot: Temperature-/Urea-Dependent Folding Kinetics and Thermodynamics**

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3864  [dx.doi.org/10.1021/jp410689m](https://doi.org/10.1021/jp410689m)


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3881  [dx.doi.org/10.1021/jp412176f](https://doi.org/10.1021/jp412176f)

**Anionic Form of Usnic Acid Promotes Lamellar to Nonlamellar Transition in DPPC and DOPC Membranes**

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3887  [dx.doi.org/10.1021/jp4124138](https://doi.org/10.1021/jp4124138)

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3893  [dx.doi.org/10.1021/jp500683n](https://doi.org/10.1021/jp500683n)

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3899  [dx.doi.org/10.1021/jp5009576](https://doi.org/10.1021/jp5009576)  
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3941  [dx.doi.org/10.1021/jp4122886](https://doi.org/10.1021/jp4122886)  
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3950  [dx.doi.org/10.1021/jp412395x](https://doi.org/10.1021/jp412395x)  
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3973 [dx.doi.org/10.1021/jp500063c](https://doi.org/10.1021/jp500063c)  
**Viscosity and Carbon Dioxide Solubility for  $\text{LiPF}_6$ ,  $\text{LiTFSI}$ , and  $\text{LiFAP}$  in Alkyl Carbonates: Lithium Salt Nature and Concentration Effect**  
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3981 [dx.doi.org/10.1021/jp500300y](https://doi.org/10.1021/jp500300y)  
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[dx.doi.org/10.1021/jp500636j](https://doi.org/10.1021/jp500636j)

**Time-Resolved IR Spectroscopy of 1,3-Dicyanophenylcyclopentane-1,3-diyl Diradicals: CN Stretching Wavenumber as a Vibrational Signature of Radical Character**

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[dx.doi.org/10.1021/jp410201t](https://doi.org/10.1021/jp410201t)

**Local Orientational Analysis of Helical Filaments and Nematic Director in a Nanoscale Phase Separation Composed of Rod-Like and Bent-Core Liquid Crystals Using Small- and Wide-Angle X-ray Microbeam Scattering**

Yoichi Takanishi,\* Haruhiko Yao, Takuya Fukasawa, Kenji Ema, Youko Ohtsuka, Yumiko Takahashi, Jun Yamamoto, Hideo Takezoe, and Atsuo Iida

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[dx.doi.org/10.1021/jp412511e](https://doi.org/10.1021/jp412511e)

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[dx.doi.org/10.1021/jp4125974](https://doi.org/10.1021/jp4125974)

**Reversed Hexagonal Lyotropic Liquid-Crystal and Open-Shell Glycodendrimers as Potential Vehicles for Sustained Release of Sodium Diclofenac**

Liron Bitan-Cherbakovsky, Dima Libster, Dietmar Appelhans, Brigitte Voit, Abraham Aserin, and Nissim Garti\*

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[dx.doi.org/10.1021/jp500650p](https://doi.org/10.1021/jp500650p)

**pH and Substrate Effect on Adsorption of Peptides Containing Z and E Dehydrophenylalanine. Surface-Enhanced Raman Spectroscopy Studies on Ag Nanocolloids and Electrodes**

Kamilla Malek,\* Agata Królikowska, and Jolanta Bukowska

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[dx.doi.org/10.1021/jp5011605](https://doi.org/10.1021/jp5011605)

**New Insights into the Thermal Stability of the Smectic C Phase**

François Porzio, Etienne Levert, Richard Vadnais, and Armand Soldera\*

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[dx.doi.org/10.1021/jp502095n](https://doi.org/10.1021/jp502095n)

**Investigation of Acrylic Acid at High Pressure Using Neutron Diffraction**

Blair F. Johnston, William G. Marshall, Simon Parsons, Andrew J. Urquhart, and Iain D. H. Oswald\*