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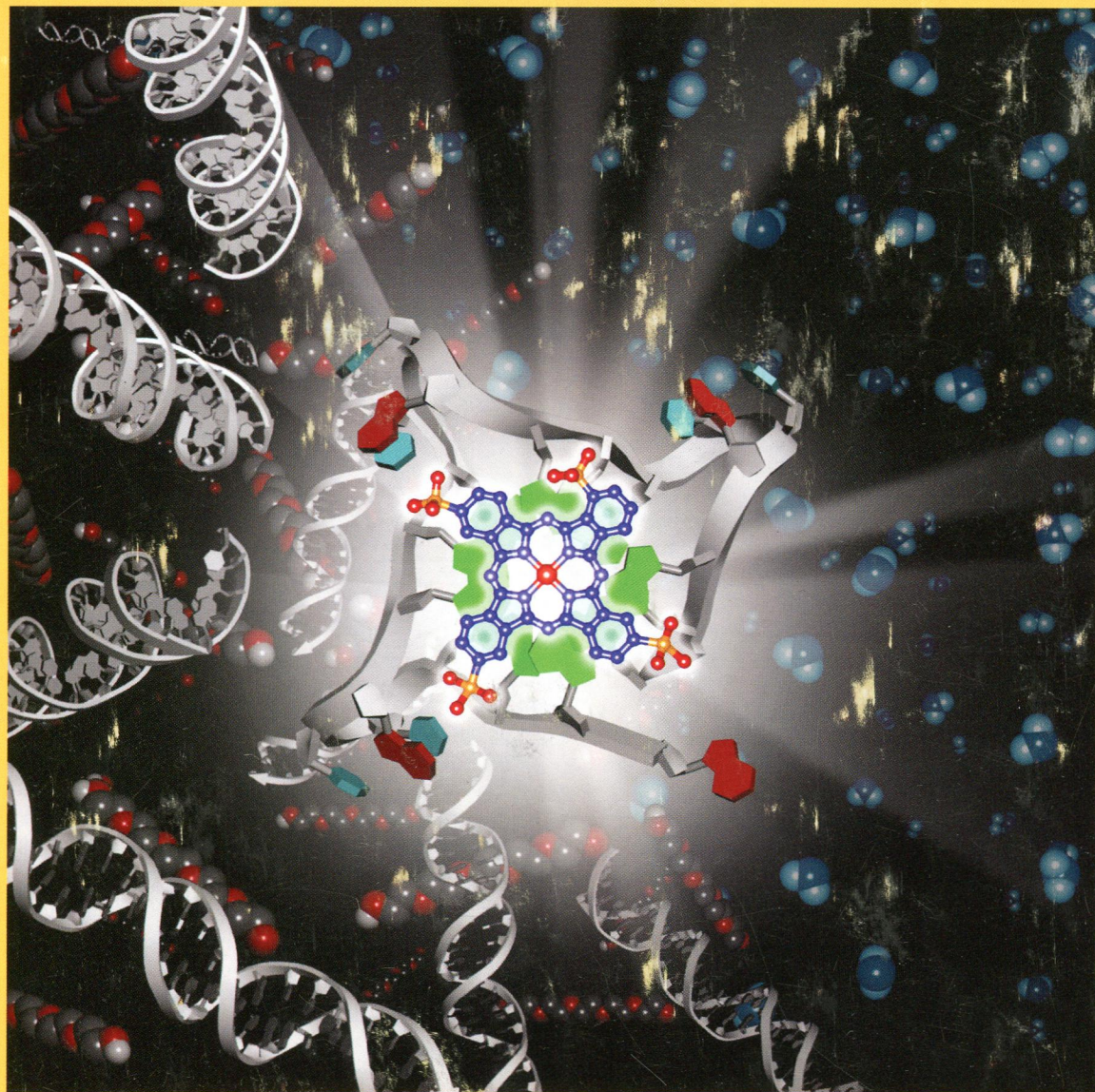
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# THE JOURNAL OF PHYSICAL CHEMISTRY

**B**

**Artificial Cell  
Nuclei-Mimicking  
Condition Predicting a  
G-Quadruplex Ligand  
Function in a Cell  
(see page 5A)**

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**ON THE COVER:** Artificial cell nuclei-mimicking condition predicting a G-quadruplex ligand function in a cell. Under an in vitro condition mimicking cell nuclei with molecular crowding reagent and double-stranded DNA, anionic phthalocyanines bind telomeric G-quadruplex and inhibit telomerase activity, which is consistent with results of cellular assays. See page 2605.

## Articles

### Biophysical Chemistry and Biomolecules

2605  [dx.doi.org/10.1021/jp410669t](https://doi.org/10.1021/jp410669t)

**In Vitro Assays Predictive of Telomerase Inhibitory Effect of G-Quadruplex Ligands in Cell Nuclei**

Hideobu Yaku, Takashi Murashima, Daisuke Miyoshi,\* and Naoki Sugimoto\*

2615  [dx.doi.org/10.1021/jp411478x](https://doi.org/10.1021/jp411478x)

**Coarse Grained Models Reveal Essential Contributions of Topological Constraints to the Conformational Free Energy of RNA Bulges**

Anthony M. Mustoe, Hashim M. Al-Hashimi, and Charles L. Brooks III\*

2628  [dx.doi.org/10.1021/jp412123h](https://doi.org/10.1021/jp412123h)

**Ping-Pong Protons: How Hydrogen-Bonding Networks Facilitate Heterolytic Bond Cleavage in Peptide Radical Cations**

Konstantin O. Zhurov, Matthew D. Wodrich, Clémence Corminboeuf, and Yury O. Tsybin\*

2638  [dx.doi.org/10.1021/jp412153s](https://doi.org/10.1021/jp412153s)

**Alzheimer's A $\beta$ 10–40 Peptide Binds and Penetrates DMPC Bilayer: An Isobaric–Isothermal Replica Exchange Molecular Dynamics Study**

Christopher Lockhart and Dmitri K. Klimov\*

2649 [dx.doi.org/10.1021/jp412373m](https://doi.org/10.1021/jp412373m)


**Nanojacketing and Dejacketing of ds-DNA: A Nondestructive Characterization of a Nanojacketed Sample by Impedance Spectroscopy**

Sudipta Nandi, Pratap Mukherjee, Aniruddha Kundu, and Arun K. Nandi\*

2662  [dx.doi.org/10.1021/jp412475u](https://doi.org/10.1021/jp412475u)

**Solvent Isotope Effect on the Dark Adaptation of Bacteriorhodopsin in Purple Membrane: Viewpoints of Kinetics and Thermodynamics**

Han-Kuei Chiang and Li-Kang Chu\*

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[dx.doi.org/10.1021/jp412600e](https://doi.org/10.1021/jp412600e)

**Translocation Thermodynamics of Linear and Cyclic Nonaarginine into Model DPPC Bilayer via Coarse-Grained Molecular Dynamics Simulation: Implications of Pore Formation and Nonadditivity**  
Yuan Hu, Xiaorong Liu, Sudipta Kumar Sinha, and Sandeep Patel\*

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[dx.doi.org/10.1021/jp500406p](https://doi.org/10.1021/jp500406p)


**Self-Assembly of Amphiphilic Peptide (AF)<sub>6</sub>H<sub>5</sub>K<sub>15</sub> Derivatives: Roles of Hydrophilic and Hydrophobic Residues**  
Naresh Thota and Jianwen Jiang\*

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[dx.doi.org/10.1021/jp500746a](https://doi.org/10.1021/jp500746a)

**Coherent Transport and Energy Flow Patterns in Photosynthesis under Incoherent Excitation**  
Kenley M. Pelzer, Tankut Can, Stephen K. Gray, Dirk K. Morr,\* and Gregory S. Engel\*

## Biomaterials, Surfactants, and Membranes

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[dx.doi.org/10.1021/jp407948p](https://doi.org/10.1021/jp407948p)

**Comparative Photoactivity and Stability of Isolated Cyanobacterial Monomeric and Trimeric Photosystem I**  
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## Liquids; Chemical and Dynamical Processes in Solution

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[dx.doi.org/10.1021/jp411904w](https://doi.org/10.1021/jp411904w)

**Free Volume Model for the Unexpected Effect of C2-Methylation on the Properties of Imidazolium Ionic Liquids**  
Zheng Jian Chen and Jong-Min Lee\*

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[dx.doi.org/10.1021/jp500137u](https://doi.org/10.1021/jp500137u)

**Solubility of Gases in a Common Ionic Liquid from Molecular Dynamics Based Free Energy Calculations**  
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[dx.doi.org/10.1021/jp500953m](https://doi.org/10.1021/jp500953m)

**On the Origin of Mesoscale Structures in Aqueous Solutions of Tertiary Butyl Alcohol: The Mystery Resolved**  
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[dx.doi.org/10.1021/jp501343k](https://doi.org/10.1021/jp501343k)

**Rotational Diffusion of Nonpolar and Charged Solutes in Propylammonium Nitrate–Propylene Glycol Mixtures: Does the Organized Structure of the Ionic Liquid Influence Solute Rotation?**  
Sugosh R. Prabhu and G. B. Dutt\*

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[dx.doi.org/10.1021/jp411612g](https://doi.org/10.1021/jp411612g)

**A Simulation Study on OH-Containing Polyimide (HPI) and Thermally Rearranged Polybenzoxazoles (TR-PBO): Relationship between Gas Transport Properties and Free Volume Morphology**

Chi Hoon Park, Elena Tocci,\* Seungju Kim, Apurva Kumar, Young Moo Lee, and Enrico Drioli

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[dx.doi.org/10.1021/jp4124056](https://doi.org/10.1021/jp4124056)

**Self-Aggregation of New Alkylcarboxylate-Based Anionic Surface Active Ionic Liquids: Experimental and Theoretical Investigations**

Ni Cheng, Pengming Yu, Tao Wang, Xiang Sheng, Yanhui Bi, Yanjun Gong, and Li Yu\*

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[dx.doi.org/10.1021/jp500672f](https://doi.org/10.1021/jp500672f)

**The Adsorption Behavior of Ionic Surfactants and Their Mixtures with Nonionic Polymers and with Polyelectrolytes of Opposite Charge at the Air–Water Interface**

Alireza Bahramian, Robert K. Thomas,\* and Jeffrey Penfold