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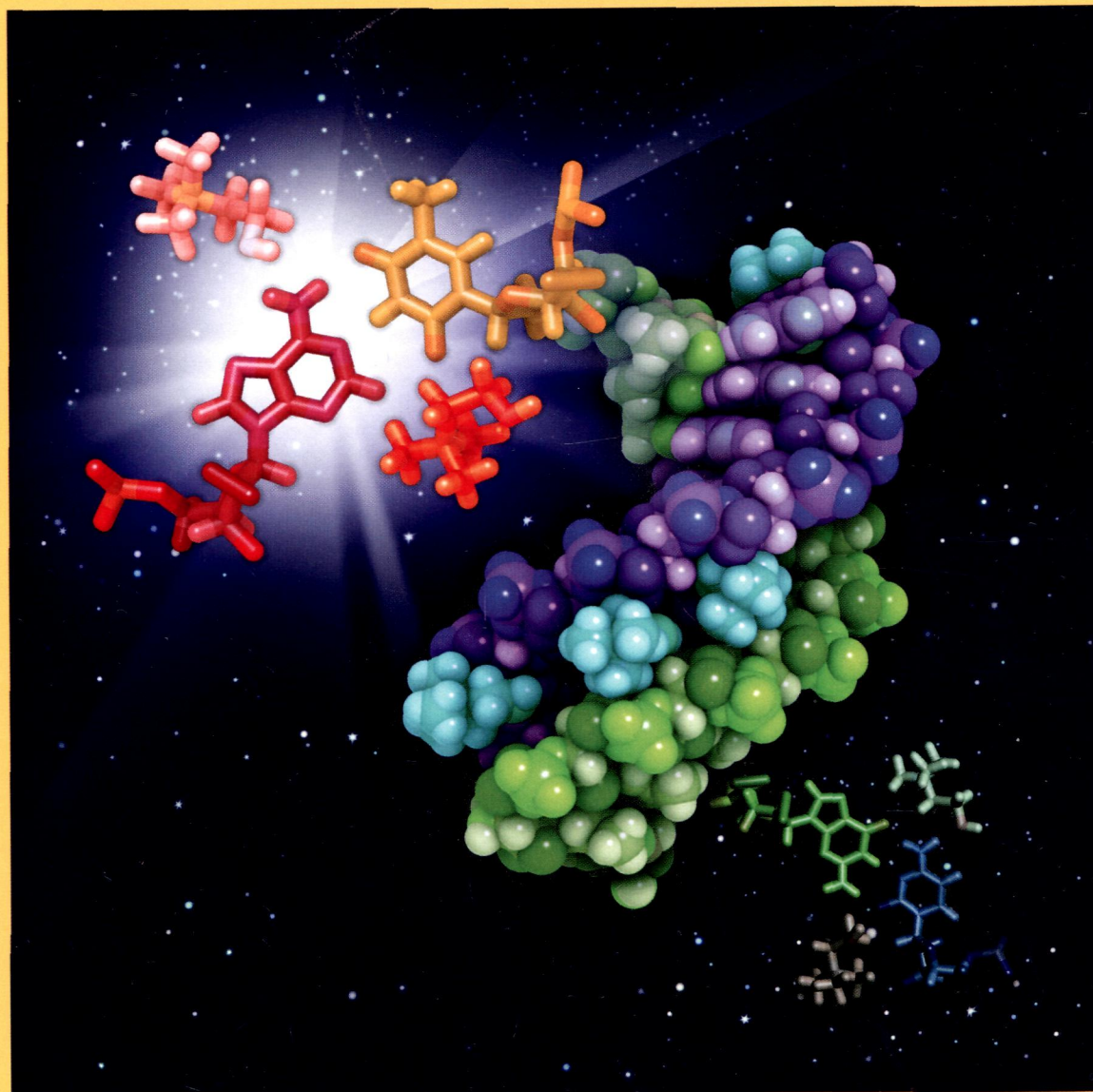
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The A–T Base Pair
Is the Most Stable
Base Pair in
Choline-Containing
Solutions
(see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: The A–T base pair is the most stable base pair in choline-containing solutions. The unique binding interactions of choline ions with DNA duplexes from a microscopic viewpoint are elucidated using molecular dynamics simulations. The choline ions bind stably through multiple hydrogen-bonding networks with DNA atoms. The affinity of the choline ion for the minor groove of the A–T base pairs is more than 2 times that for other groove areas. In the narrow A–T minor groove, the choline ion has high affinity for the ribose atoms of thymine. In contrast, choline ions break the formation of hydrogen bonds between G–C base pairs by binding to the base atoms. Therefore, in a solution containing choline ions, A–T base pairs are more stable than G–C base pairs because of preferential binding of the choline ions to the DNA duplexes. See page 379.

Articles

Biophysical Chemistry and Biomolecules


- 379  [dx.doi.org/10.1021/jp406647b](https://doi.org/10.1021/jp406647b)
Choline Ion Interactions with DNA Atoms Explain Unique Stabilization of A–T Base Pairs in DNA Duplexes: A Microscopic View
 Miki Nakano, Hisae Tateishi-Karimata, Shigenori Tanaka, and Naoki Sugimoto*


- 390  [dx.doi.org/10.1021/jp407365x](https://doi.org/10.1021/jp407365x)
Enolization as an Alternative Proton Delivery Pathway in Human Aromatase (P450 19A1)
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- 406  [dx.doi.org/10.1021/jp408061k](https://doi.org/10.1021/jp408061k)
Quantitative Evaluation of Myoglobin Unfolding in the Presence of Guanidinium Hydrochloride and Ionic Liquids in Solution
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- 413 [dx.doi.org/10.1021/jp408234k](https://doi.org/10.1021/jp408234k)
Correlated Dynamical Crossovers of the Hydration Layer of a Single-Stranded DNA Oligomer
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- 423  [dx.doi.org/10.1021/jp408293k](https://doi.org/10.1021/jp408293k)
RNA Polymerase II Subunits Exhibit a Broad Distribution of Macromolecular Assembly States in the Interchromatin Space of Cell Nuclei
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434  [dx.doi.org/10.1021/jp408536s](https://doi.org/10.1021/jp408536s)
Computational Evaluations of Charge Coupling and Hydrogen Bonding in the Active Site of a Family 7 Cellobiohydrolase
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Noncovalent Interactions in Microsolvated Networks of Trimethylamine *N*-Oxide
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460  [dx.doi.org/10.1021/jp409491d](https://doi.org/10.1021/jp409491d)
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Computational Studies of the Regioselectivities of COMT-Catalyzed *Meta*-/*Para*-O Methylations of Luteolin and Quercetin
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Model Study Using Designed Selenopeptides on the Importance of the Catalytic Triad for the Antioxidative Functions of Glutathione Peroxidase
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Familial Alzheimer A2 V Mutation Reduces the Intrinsic Disorder and Completely Changes the Free Energy Landscape of the A β 1–28 Monomer
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Biomaterials, Surfactants, and Membranes


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The Tunable Hydrophobic Effect on Electrically Doped Graphene
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Ethanol-Induced Perturbations to Planar Lipid Bilayer Structures
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Dielectric Properties of Water Ice, the Ice Ih/XI Phase Transition, and an Assessment of Density Functional Theory
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Molecular Dynamics of DNA–Protein Conjugates on Electrified Surfaces: Solutions to the Drift-Diffusion Equation
A. Langer, W. Kaiser, M. Svejda, P. Schwertler, and U. Rant*

Glasses, Colloids, Polymers, and Soft Matter

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Self-Oscillation of Polymer Chains with an Fe(bpy)₃ Catalyst Induced by the Belousov–Zhabotinsky Reaction
Yusuke Hara,* Kenji Fujimoto, and Hiroyuki Mayama

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[dx.doi.org/10.1021/jp409577y](https://doi.org/10.1021/jp409577y)**Self-Assembly of Poly(1,4-phenylene-[9,9-bis(4-phenoxy-butylsulfonate)]fluorene-2,7-diyl) with Oppositely Charged Phenylenevinylene Oligoelectrolytes**

Telma Costa,* Ana T. Marques, J. Sérgio Seixas de Melo, Alexander W. Thomas, Logan E. Garner, Ullrich Scherf, Guillermo C. Bazan, and Hugh D. Burrows

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[dx.doi.org/10.1021/jp410448y](https://doi.org/10.1021/jp410448y)**Vibrational Density of States and Elastic Properties of Cross-Linked Polymers: Combining Inelastic Light and Neutron Scattering**

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[dx.doi.org/10.1021/jp410915p](https://doi.org/10.1021/jp410915p)**Switching the BZ Reaction with a Strong-Acid-Free Gel**

Yusuke Hara,* Yoshinori Yamaguchi, and Hiroyuki Mayama

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[dx.doi.org/10.1021/jp410934g](https://doi.org/10.1021/jp410934g)**Non-Exponential Kinetics and a Complete Folding Pathway of an α -Helical Heteropeptide: Direct Observation and Comprehensive Molecular Dynamics**

Gouri S. Jas,* C. Russell Middaugh, and Krzysztof Kuczera

Additions and Corrections

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[dx.doi.org/10.1021/jp4120404](https://doi.org/10.1021/jp4120404)**Correction to "Relaxation of Bulk Metallic Glasses Studied by Mechanical Spectroscopy"**

Jichao Qiao, Jean-Marc Pelletier,* and Riccardo Casalini