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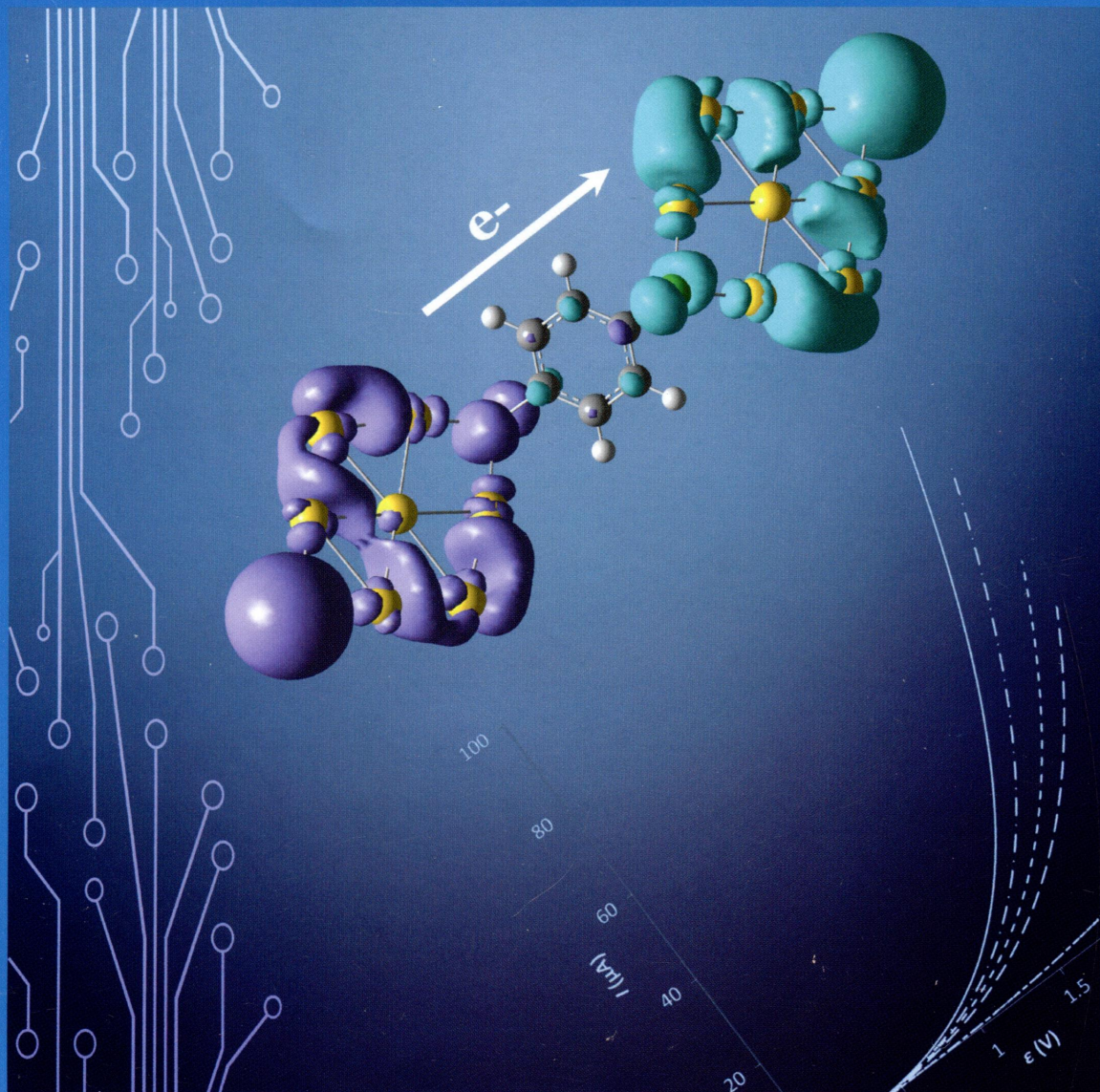
NUMBER 21

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THE JOURNAL OF
PHYSICAL
CHEMISTRY

A

Electron Transfer
Induced by an
External Electric
Voltage
(see page 3827)



ISOLATED MOLECULES, CLUSTERS, RADICALS, AND IONS; ENVIRONMENTAL CHEMISTRY,
GEOCHEMISTRY, AND ASTROCHEMISTRY; THEORY



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ON THE COVER: Interfacial structure dictated by interplay among adsorbed molecule, solvent, and substrate features. The complexity of the solid-liquid interface is attributed to the orientation and conformation of adsorbed molecules, the structure of the interfacial solvent, and the nature of the substrate surface. A combination of experimental and modeling efforts may be applied to shed light on this chemically and physically unique environment. See page 5617.

Feature Article

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dx.doi.org/10.1021/jp412742u

Molecular-Level Surface Structure from Nonlinear Vibrational Spectroscopy Combined with Simulations

Shaun A. Hall, Kailash C. Jena, Paul A. Covert, Sandra Roy, Travis G. Trudeau, and Dennis K. Hore*

Articles

Biophysical Chemistry and Biomolecules

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dx.doi.org/10.1021/jp412743s

Pyroglutamylated Amyloid- β Peptide Reverses Cross β -Sheets by a Prion-Like Mechanism

Jason O. Matos, Greg Goldblatt, Jaekyun Jeon, Bo Chen, and Suren A. Tatulian*

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dx.doi.org/10.1021/jp501228s

Reaction Mechanism of Zinc-Dependent Cytosine Deaminase from *Escherichia coli*: A Quantum-Chemical Study

Bianca Manta, Frank M. Raushel, and Fahmi Himo*

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dx.doi.org/10.1021/jp502069a

Aromatic Interactions Modulate the 5'-Base Selectivity of the DNA-Binding Autoantibody ED-10

Yi An, Rajesh K. Raju, Tongxiang Lu, and Steven E. Wheeler*

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dx.doi.org/10.1021/jp5022664

Shear-Stress-Induced Conformational Changes of von Willebrand Factor in a Water–Glycerol Mixture Observed with Single Molecule Microscopy

Robrecht M. A. Vergauwe, Hiroshi Uji-i, Karen De Ceunynck, Jan Vermant, Karen Vanhoorelbeke, and Johan Hofkens*

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dx.doi.org/10.1021/jp5023482

Molecular Structures of C- and N-Terminus Cysteine Modified Cecropin P1 Chemically Immobilized onto Maleimide-Terminated Self-Assembled Monolayers Investigated by Molecular Dynamics Simulation

Zunliang Wang, Xiaofeng Han, Nongyue He,* Zhan Chen,* and Charles L. Brooks III*

5681  [dx.doi.org/10.1021/jp502664a](https://doi.org/10.1021/jp502664a)
Relationship between Nonlinear Pressure-Induced Chemical Shift Changes and Thermodynamic Parameters
Markus Beck Erlach, Joerg Koehler, Beate Moeser, Dominik Horinek, Werner Kremer, and Hans Robert Kalbitzer*

5691  [dx.doi.org/10.1021/jp5037348](https://doi.org/10.1021/jp5037348)
Comparative Study of Protein Folding in Aqueous Urea and Dimethyl Sulfoxide Solutions: Surface Polarity, Solvent Specificity, and Sequence of Secondary Structure Melting
Susmita Roy and Biman Bagchi*

Biomaterials, Surfactants, and Membranes

5698  [dx.doi.org/10.1021/jp500139p](https://doi.org/10.1021/jp500139p)
Temperature and Pressure Based NMR Studies of Detergent Micelle Phase Equilibria
Rohan Alvares, Shaan Gupta, Peter M. Macdonald, and R. Scott Prosser*

5707 [dx.doi.org/10.1021/jp5025894](https://doi.org/10.1021/jp5025894)
Green Synthesis of Reduced Graphene Oxide/Polyaniline Composite and Its Application for Salt Rejection by Polysulfone-Based Composite Membranes
Ilker Akin, Erhan Zor, Haluk Bingol,* and Mustafa Ersoz

Liquids; Chemical and Dynamical Processes in Solution

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Theoretical Study on Two-Step Mechanisms of Peptide Release in the Ribosome
Carles Acosta-Silva, Joan Bertran,* Vicenç Branchadell, and Antoni Oliva

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Theoretical Prediction of pK_a in Methanol: Testing SM8 and SMD Models for Carboxylic Acids, Phenols, and Amines
Elizabeth L. M. Miguel, Poliana L. Silva, and Josefredo R. Pliego*

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Chemically Tunable Ionic Liquids with Aprotic Heterocyclic Anion (AHA) for CO₂ Capture
Samuel Seo, Mauricio Quiroz-Guzman, M. Aruni DeSilva, Tae Bum Lee, Yong Huang, Brett F. Goodrich, William F. Schneider, and Joan F. Brennecke*

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Quantitative Analysis of Conductivity and Viscosity of Ionic Liquids in Terms of Their Relaxation Times
Tsuayoshi Yamaguchi,* Eiichi Nakahara, and Shinobu Koda

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Ultrafast Dynamics of C30 in Solution and within CDs and HSA Protein
Cristina Martin, Boiko Cohen, Issam Gaamoussi, Mustapha Ijjaali, and Abderrazzak Douhal*

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[dx.doi.org/10.1021/jp503130y](https://doi.org/10.1021/jp503130y)

Charge Templates in Aromatic Plus Ionic Liquid Systems Revisited: NMR Experiments and Molecular Dynamics Simulations
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[dx.doi.org/10.1021/jp503285w](https://doi.org/10.1021/jp503285w)

Simultaneous Detection of Images and Raman Spectra of Colliding Droplets: Composition Analysis of Protrusions Emerging during Collisions of Ethanol and Water Droplets
Tomoko Suzuki and Jun-ya Kohno*

Glasses, Colloids, Polymers, and Soft Matter

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[dx.doi.org/10.1021/jp502987a](https://doi.org/10.1021/jp502987a)

Ion Solvation in Polymer Blends and Block Copolymer Melts: Effects of Chain Length and Connectivity on the Reorganization of Dipoles
Issei Nakamura*

Additions and Corrections

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[dx.doi.org/10.1021/jp5045755](https://doi.org/10.1021/jp5045755)

Correction to "Direct Observation of Vibrational Energy Flow in Cytochrome c"
Naoki Fujii, Misao Mizuno, and Yasuhisa Mizutani*