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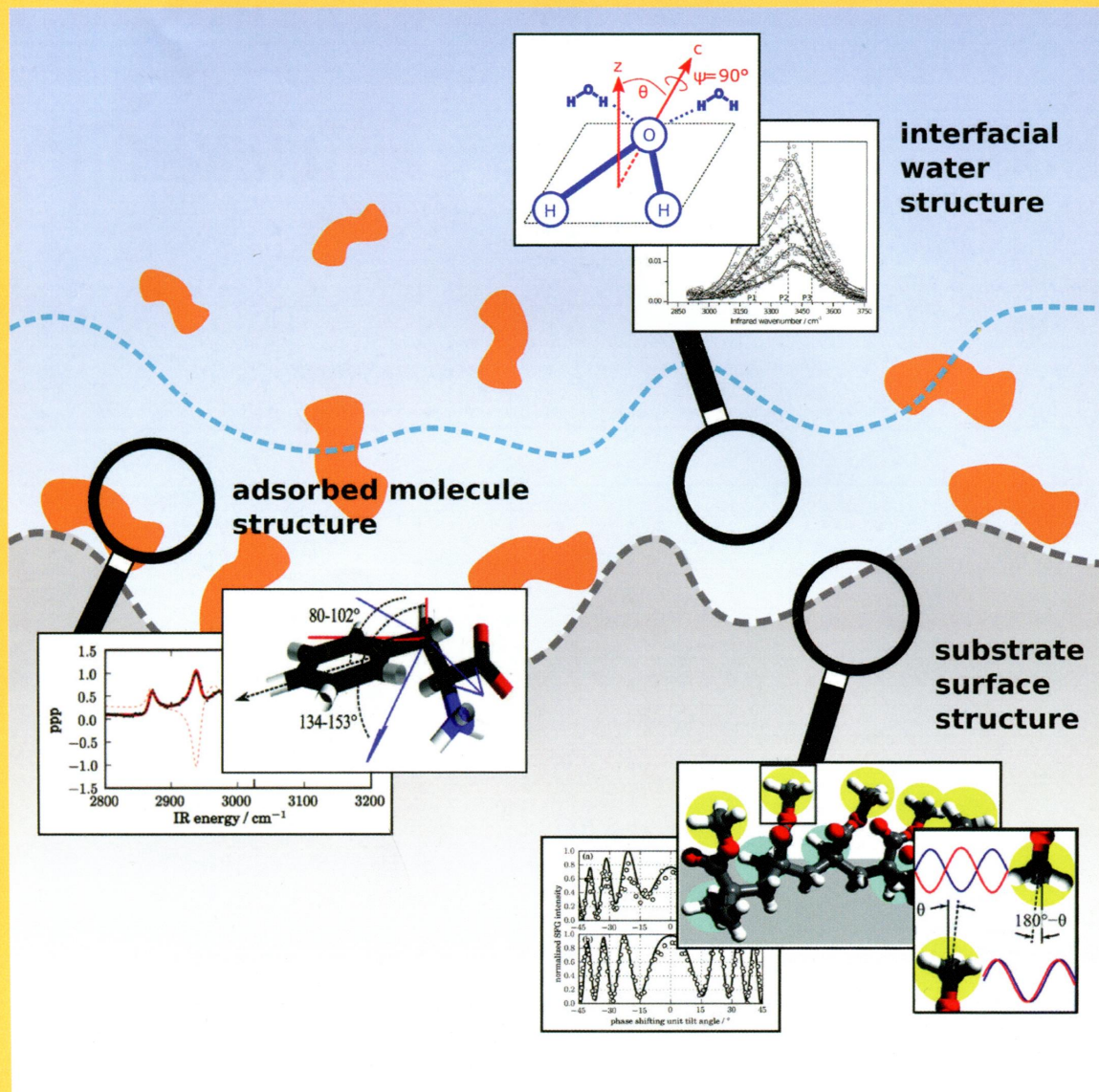
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B



Interfacial Structure Dictated by Interplay among Adsorbed Molecule, Solvent, and Substrate Features
(see page 5617)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: The development of simple methodologies for the calculation of the electric conductance plays an important role within the field of molecular electronics. Here, the I/V profiles of benzene-1,4-dithiolate directly attached to gold clusters of different size arranged in bridge and top conformations have been determined by a revisited approach based on the uncertainty principle. The electric response has been analyzed using electron deformation orbitals (EDOs). The main EDOs in a bridge conformation are represented in the figure showing the effective electron transfer upon an external voltage of 2.5 V. See page 3827.

Articles

Kinetics and Dynamics

3711

[dx.doi.org/10.1021/jp501516k](https://doi.org/10.1021/jp501516k)
Kinetic Studies on the Synthesis of Monoclinic $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ via Solid-State Reaction

Shanhua Chen,* Jun Wu, Zelong Su, and Ling Deng

Spectroscopy, Photochemistry, and Excited States

3717


[dx.doi.org/10.1021/jp503831p](https://doi.org/10.1021/jp503831p)
Light-Induced Structural Change in Iridium Complexes Studied by Electron Spin Resonance

A. Batagin-Neto, A. P. Assis, J. F. Lima, C. J. Magon, L. Yan, M. Shao, B. Hu, and C. F. O. Graeff*

3726

[dx.doi.org/10.1021/jp4118002](https://doi.org/10.1021/jp4118002)
Infrared Absorption Spectra of Jahn–Teller Systems: Application to the Transition-Metal Trifluorides MnF_3 and NiF_3

Padmabati Mondal* and Wolfgang Domcke

3735


[dx.doi.org/10.1021/jp500260f](https://doi.org/10.1021/jp500260f)
Synchrotron Photoionization Study of Mesitylene Oxidation Initiated by Reaction with $\text{Cl}(^2\text{P})$ or $\text{O}(^3\text{P})$ Radicals

Martin Y. Ng, Jordan Nelson, Craig A. Taatjes, David L. Osborn, and Giovanni Meloni*

3749

[dx.doi.org/10.1021/jp5009658](https://doi.org/10.1021/jp5009658)
Symmetry Breaking in Platinum Acetylide Chromophores Studied by Femtosecond Two-Photon Absorption Spectroscopy

Aleksander Rebane,* Mikhail Drobizhev, Nikolay S. Makarov, Geoffrey Wicks, Pawel Wnuk, Yuriy Stepanenko, Joy E. Haley, Douglas M. Krein, Jennifer L. Fore, Aaron R. Burke, Jonathan E. Slagle, Daniel G. McLean, and Thomas M. Cooper*

3760


[dx.doi.org/10.1021/jp5021966](https://doi.org/10.1021/jp5021966)
Substituent and Solvent Effects on the Absorption Spectra of Cation– π Complexes of Benzene and Borazine: A Theoretical Study

Nabajit Sarmah, Pradip Kr. Bhattacharyya,* and Kusum K. Bania*

3775 [dx.doi.org/10.1021/jp502406u](https://doi.org/10.1021/jp502406u)**Spectral and Kinetic Properties of Radical Cations Derived from Oxoisoaporphines: Relevance to Electron-Transfer Processes Involving Phytoalexins**

Julio R. De la Fuente,* Gabriel Kciuk, Christian Aliaga, and Krzysztof Bobrowski*

3787 [dx.doi.org/10.1021/jp502833c](https://doi.org/10.1021/jp502833c)**Effect of Proton Substitution by Alkali Ions on the Fluorescence Emission of Rhodamine B Cations in the Gas Phase**


Jean-François Greisch,* Michael E. Harding, Wim Klopper, Manfred M. Kappes, and Detlef Schooss*

3795 [dx.doi.org/10.1021/jp5029245](https://doi.org/10.1021/jp5029245)**Persistent Intramolecular C–H...X (X = O or S) Hydrogen-Bonding in Benzyl Meldrum's Acid Derivatives**


W. Scott Hopkins,* Moaraj Hasan, Michael Burt, Rick A. Marta, Eric Fillion, and Terry B. McMahon

3804 [dx.doi.org/10.1021/jp5038969](https://doi.org/10.1021/jp5038969)**Gas Phase Structure of Metal Mediated (Cytosine)₂Ag⁺ Mimics the Hemiprotonated (Cytosine)₂H⁺ Dimer in *i*-Motif Folding**

Matias Berdakin, Vincent Steinmetz, Philippe Maitre, and Gustavo A. Pino*

Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry3810 [dx.doi.org/10.1021/jp501595n](https://doi.org/10.1021/jp501595n)**Gas-Phase Synthesis of Boronyllallene (H₂CCCH(BO)) under Single Collision Conditions: A Crossed Molecular Beams and Computational Study**

Surajit Maity, Dorian S. N. Parker, Ralf I. Kaiser,* Brad Ganoe, Stefan Fau, Ajith Perera, and Rodney J. Bartlett*

Molecular Structure, Quantum Chemistry, and General Theory3820 [dx.doi.org/10.1021/jp5003929](https://doi.org/10.1021/jp5003929)**Experimental and Computational Thermochemistry of 3- and 4-Nitrophthalic Anhydride**

Miguel A. García-Castro, Patricia Amador,* Julio M. Hernández-Pérez, Adrián E. Medina-Favela, and Henoc Flores

3827

[dx.doi.org/10.1021/jp501485a](https://doi.org/10.1021/jp501485a)**Revisiting the Calculation of *I/V* Profiles in Molecular Junctions Using the Uncertainty Principle**

Nicolás Ramos-Berdullas and Marcos Mandado*

3835 [dx.doi.org/10.1021/jp501932g](https://doi.org/10.1021/jp501932g)**Substituent Effects in the Noncovalent Bonding of SO₂ to Molecules Containing a Carbonyl Group. The Dominating Role of the Chalcogen Bond**

Luis Miguel Azofra and Steve Scheiner*

Why Is the L-Shaped Structure of $X_2 \cdots X_2$ ($X = F, Cl, Br, I$) Complexes More Stable Than Other Structures?

Robert Sedlak, Palanisamy Deepa, and Pavel Hobza*