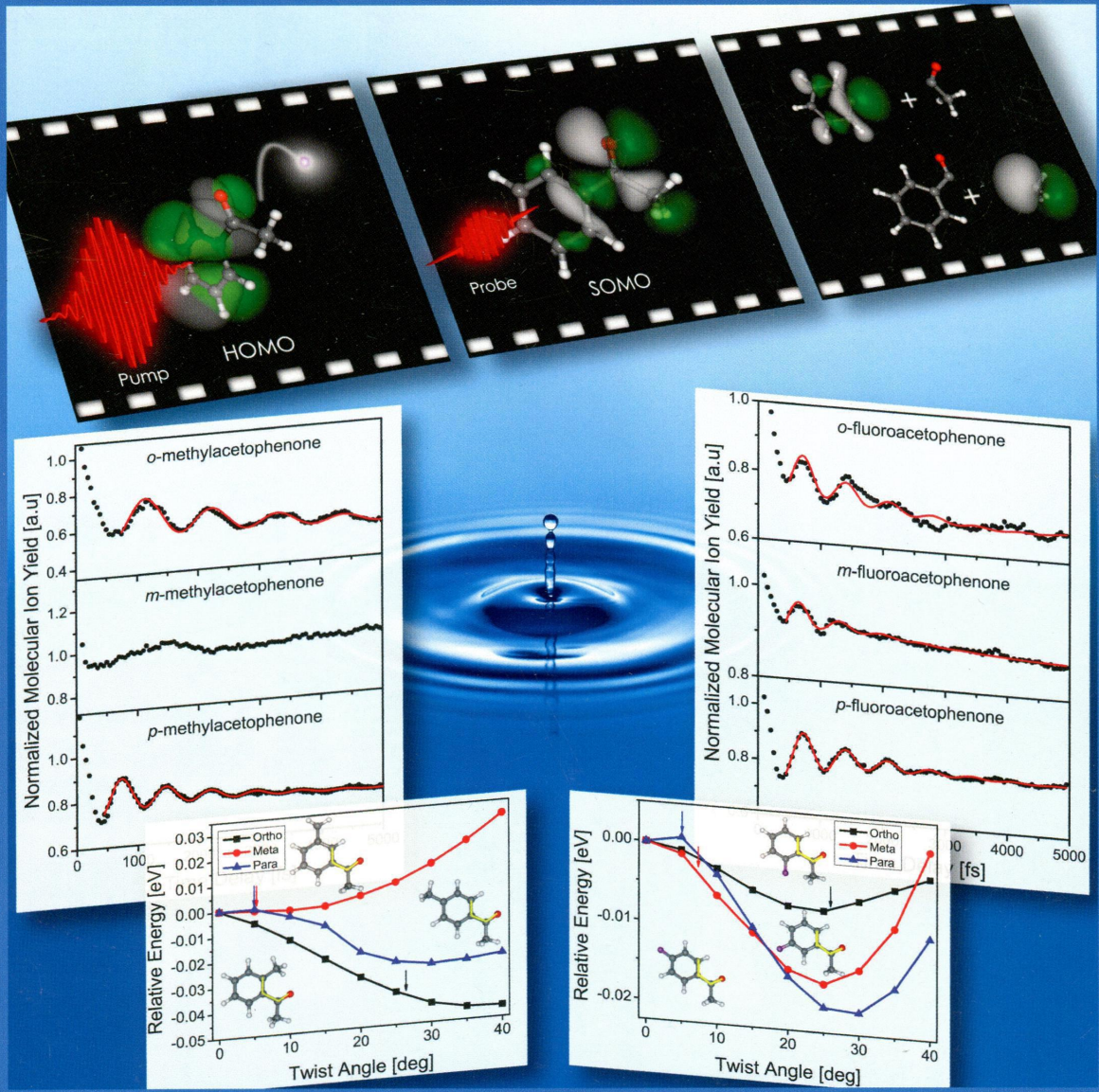


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Polyatomic Molecules Being Ionized by Strong Laser Fields Do Not Behave Like a "Bag of Atoms" (see page 11433)

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

ON THE COVER: Photoelectron carries most of the energy during femtosecond strong-field ionization of large molecules. Intense laser–molecule interactions lead to ionization and fragmentation, but a definitive and predictive mechanistic interpretation of these processes has been elusive. The cover symbolizes our approach and key conclusions in work to understand this problem. We study the dynamical behavior of a group of alkyl phenyl ketones using time-of-flight mass spectroscopy in conjunction with strong-field ionization pump pulses followed by weak probe pulses. The ion yields reveal temporal modulations due to low-energy (milli-electronvolt) conformational motions post ionization. Our results are supported by high level *ab initio* calculations and find that the most polarizable electron is ejected from the HOMO, taking away most of the energy, and leaving a relatively cold cation, analogous to a single water drop rebounding after drops have entered a water surface. Further fragmentation depends on the electronic distribution of the SOMO and the presence of resonances in the cationic excited states. We conclude that even in intense laser fields, volts per Angstrom, molecules and ions cannot be viewed as easily scrambled “bags of atoms”; instead, they show substituent effects easily rationalized in traditional organic chemistry terms. See page 11433.

Feature Article

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Polyatomic Molecules under Intense Femtosecond Laser Irradiation

Arkaprabha Konar, Yinan Shu, Vadim V. Lozovoy, James E. Jackson, Benjamin G. Levine, and Marcos Dantus*

Articles


Kinetics and Dynamics

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DOI: 10.1021/jp507459m

Multisurface Multimode Molecular Dynamical Simulation of Naphthalene and Anthracene Radical Cations by Using Nearly Linear Scalable Time-Dependent Discrete Variable Representation Method


Basir Ahamed Khan, Subhankar Sardar,* Pranab Sarkar, and Satrajit Adhikari

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DOI: 10.1021/jp508731q

Prediction of Crystal Morphology of Cyclotrimethylene Trinitramine in the Solvent Medium by Computer Simulation: A Case of Cyclohexanone Solvent

Gang Chen, Mingzhu Xia,* Wu Lei, Fengyun Wang, and Xuedong Gong

11479 

DOI: 10.1021/jp5096618

Elucidation of Electron Ionization Induced Fragmentations of Adenine by Semiempirical and Density Functional Molecular Dynamics

Christoph Alexander Bauer and Stefan Grimme*

11485

DOI: 10.1021/jp510399v

Experimental and Theoretical Kinetics for the $\text{H}_2\text{O}^+ + \text{H}_2/\text{D}_2 \rightarrow \text{H}_3\text{O}^+/\text{H}_2\text{DO}^+ + \text{H/D}$ Reactions: Observation of the Rotational Effect in the Temperature Dependence

Shaun G. Ard, Anyang Li, Oscar Martinez Jr., Nicholas S. Shuman, Albert A. Viggiano,* and Hua Guo*

Spectroscopy, Photochemistry, and Excited States

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DOI: 10.1021/jp505299p

Coupled States in Dinitrofluorene: Relationships between Ground State and Excited State Mixed Valence

Matthew D. Kiesz, Ryan M. Hoekstra, Yen-Ting Chen, João P. Telo, Stephen F. Nelsen, and Jeffrey I. Zink*

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DOI: 10.1021/jp509253e

A Theoretical Study on Trivalent Europium: From the Free Ion to the Water Complex

Christof Holzer, Anna M. Wernbacher, Jan M. Senekowitsch, Karl Gatterer, and Anne-Marie Kelterer*

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DOI: 10.1021/jp5094806

Investigation of the Fluorescence Quenching of 1-Aminoanthracene by Dissolved Oxygen in Cyclohexane

Todd Pagano,* Nelsy Carcamo, and Jonathan E. Kenny

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DOI: 10.1021/jp509502w

Squaranes: Crystal Structures and Spectroscopic Analysis of Hydrated and Anhydrous Forms of Squaric Acid-Isoniazid Species

Felipe D. dos Reis, Isabela C. Gatti, Humberto C. Garcia, Vanessa E. de Oliveira, and Luiz F. C. de Oliveira*

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DOI: 10.1021/jp510517z

Vibrational Cooling Dynamics of a [FeFe]-Hydrogenase Mimic Probed by Time-Resolved Infrared Spectroscopy

Benjamin W. Caplins, Justin P. Lomont, Son C. Nguyen, and Charles B. Harris*

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DOI: 10.1021/jp5113125

Chiral Asymmetry in the Multiphoton Ionization of Methyloxirane Using Femtosecond Electron–Ion Coincidence Imaging

Mohammad M. Rafiee Fanoodeh, Ivan Powis,* and Maurice H. M. Janssen

Environmental and Atmospheric Chemistry, Aerosol Processes, Geochemistry, and Astrochemistry


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DOI: 10.1021/jp507769b


Activation Barriers in the Growth of Molecular Clusters Derived from Sulfuric Acid and Ammonia


Joseph W. DePalma, Bryan R. Bzdek, Douglas P. Ridge, and Murray V. Johnston*


11555  DOI: 10.1021/jp508378z
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11572 DOI: 10.1021/jp5094959
Experimental and Computational Study of CO₂ Storage and Sequestration with Aqueous 2-Amino-2-hydroxymethyl-1,3-propanediol (TRIS) Solutions
Rama Oktavian, Mohamed Taha,* and Ming-Jer Lee*


Molecular Structure, Quantum Chemistry, and General Theory

11583  DOI: 10.1021/jp506601e
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11591  DOI: 10.1021/jp507309m
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11602  DOI: 10.1021/jp507312y
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11612 DOI: 10.1021/jp508330r
Stability of the Guanine Endoperoxide Intermediate: A Computational Challenge for Density Functional Theory
Raymond Grüber, Antonio Monari, and Elise Dumont*

11620  DOI: 10.1021/jp5084407
Solvation Effects on Chemical Shifts by Embedded Cluster Integral Equation Theory
Roland Frach and Stefan M. Kast*

11629 DOI: 10.1021/jp5086729
Gas-Phase Solvation of Protonated Amino Acids by Methanol
Kris Eldridge, Ronghu Wu, Jonathan K. Martens, and Terry B. McMahon*

11641  DOI: 10.1021/jp510118p
C–C Stretching Raman Spectra and Stabilities of Hydrocarbon Molecules in Natural Gas Hydrates: A Quantum Chemical Study
Yuan Liu and Lars Ojamäe*

11652

DOI: 10.1021/jp511751d

Correction to "Pulse Radiolysis Studies of 3,5-Dimethyl Pyrazole Derivatives of Selenoethers"

Atanu Barik,* Beena G. Singh, Asmita Sharma, Vimal K. Jain, and K. Indira Priyadarini

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