

JANUARY 22, 2015

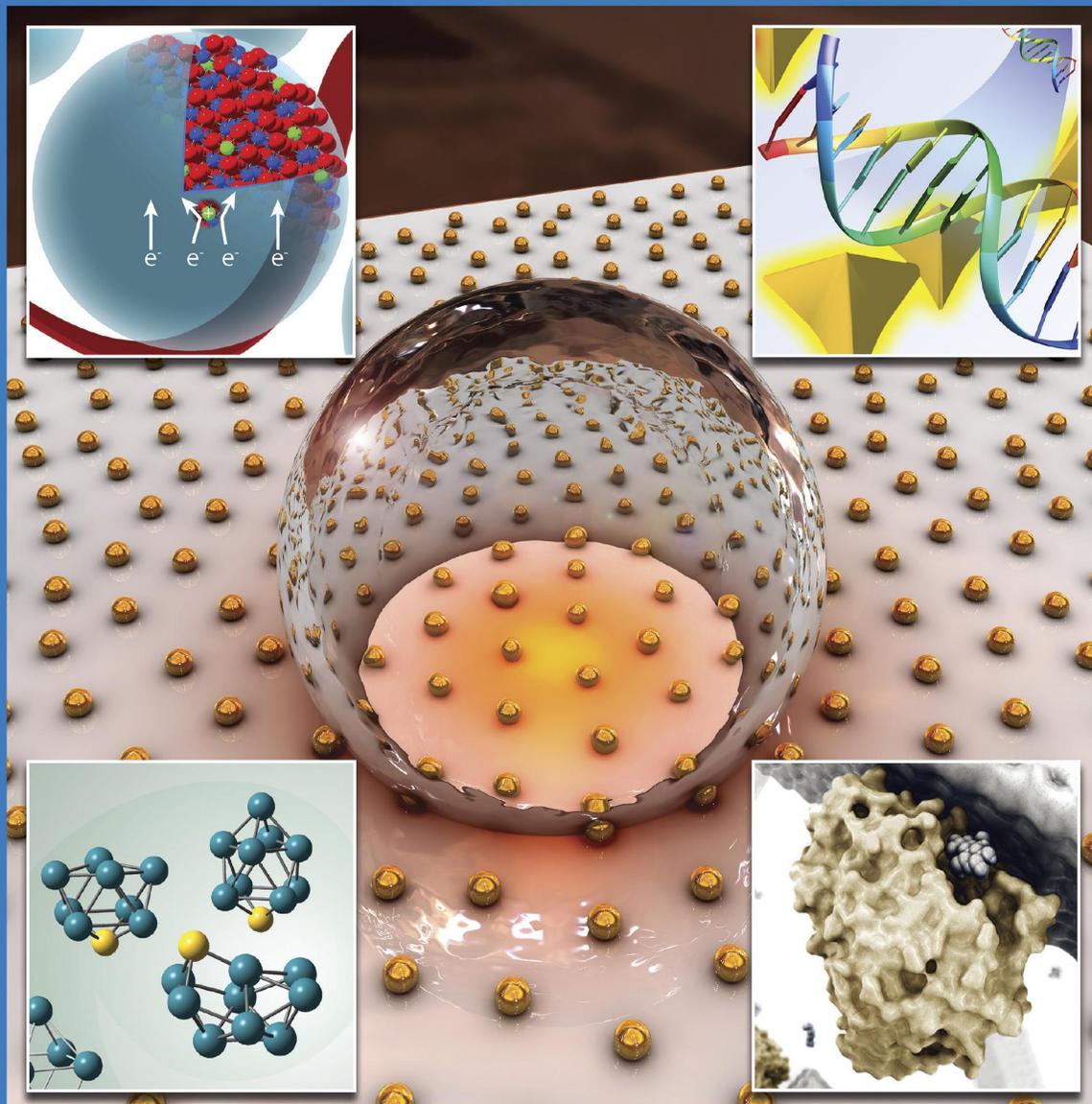
VOLUME 119

NUMBER 3

pubs.acs.org/JPCA

THE JOURNAL OF PHYSICAL CHEMISTRY

A



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



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

January 22, 2015: Vol. 119, Iss. 3

Content

1. Evaluated Kinetics of Terminal and Non-Terminal Addition of Hydrogen Atoms to 1-Alkenes: A Shock Tube Study of H + 1-Butene

Jeffrey A. Manion and Iftikhar A. Awan

The Journal of Physical Chemistry A 2015 119 (3), 429-441

2. Photoisomerization of Silyl-Substituted Cyclobutadiene Induced by $\sigma \rightarrow \pi^*$ Excitation: A Computational Study

Zexing Qu, Chen Yang, and Chungen Liu

The Journal of Physical Chemistry A 2015 119 (3), 442-451

3. Motion of Br₂ Molecules in Clathrate Cages. A Computational Study of the Dynamic Effects on Its Spectroscopic Behavior

M. I. Bernal-Uruchurtu, Kenneth C. Janda, and R. Hernández-Lamonedá

The Journal of Physical Chemistry A 2015 119 (3), 452-459

4. Strong-Field Ionization of Flash Pyrolysis Reaction Products

Fadia Cudry, James M. Oldham, Steven Lingenfelter, and Arthur G. Suits

The Journal of Physical Chemistry A 2015 119 (3), 460-467

5. Switching of the Triplet–Triplet–Annihilation Upconversion with Photoresponsive Triplet Energy Acceptor: Photocontrollable Singlet/Triplet Energy Transfer and Electron Transfer

Kejing Xu, Jianzhang Zhao, Xiaoneng Cui, and Jie Ma

The Journal of Physical Chemistry A 2015 119 (3), 468-481

6. Two-Dimensional Nuclear Magnetic Resonance: Exploiting Spin Echoes To Maximize Information Content by Suppression of Diagonal Peaks in Homonuclear Experiments

Abhishek Banerjee and Narayanan Chandrakumar

The Journal of Physical Chemistry A 2015 119 (3), 482-487

7. Thermodynamics of Small Alkali Metal Halide Cluster Ions: Comparison of Classical Molecular Simulations with Experiment and Quantum Chemistry

Lukas Vlcek, Filip Uhlík, Filip Moučka, Ivo Nezbeda, and Ariel A. Chialvo
The Journal of Physical Chemistry A **2015** 119 (3), 488-500

8. Bimolecular Decomposition Pathways for Carboxylic Acids of Relevance to Biofuels

Jared M. Clark, Mark R. Nimlos, and David J. Robichaud
The Journal of Physical Chemistry A **2015** 119 (3), 501-516

9. Interpretation of the Longitudinal ^{13}C Nuclear Spin Relaxation and Chemical Shift Data for Five Bromoazaheterocycles Supported by Nonrelativistic and Relativistic DFT Calculations

Artur Wodyński, Anna Kraska-Dziadecka, Dominika Kubica, and Adam Gryff-Keller
The Journal of Physical Chemistry A **2015** 119 (3), 517-524

10. Rethinking Aromaticity in H-Bonded Systems. Caveats for Transition Structures Involving Hydrogen Transfer and π -Delocalization

María P. Romero-Fernández, Martín Ávalos, Reyes Babiano, Pedro Cintas, José L. Jiménez, and Juan C. Palacios
The Journal of Physical Chemistry A **2015** 119 (3), 525-534

11. Chalcogen Bonds in Complexes of SOXY (X, Y = F, Cl) with Nitrogen Bases

Luis Miguel Azofra, Ibon Alkorta, and Steve Scheiner
The Journal of Physical Chemistry A **2015** 119 (3), 535-541