

FEBRUARY 19, 2015

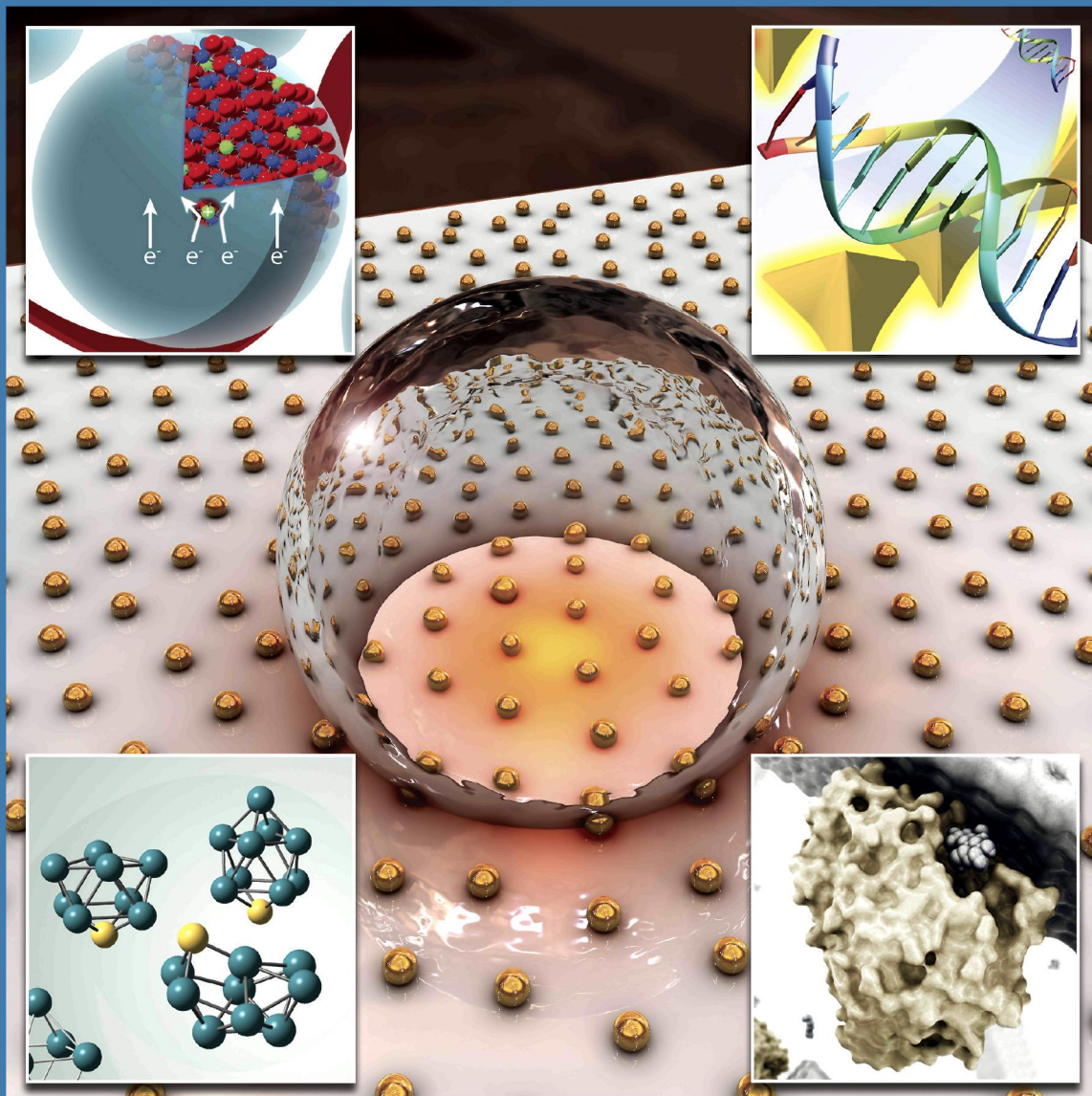
VOLUME 119

NUMBER 7

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

Content

- 1. Relationship between Activation Volume and Polymer Matrix Effects on Photochromic Performance: Bridging Molecular Parameter to Macroscale Effect**
Kentaro Shima, Katsuya Mutoh, Yoichi Kobayashi, and Jiro Abe
The Journal of Physical Chemistry A 2015 119 (7), 1087-1093
DOI: 10.1021/jp511074y
- 2. Combined Crossed Molecular Beam and Ab Initio Investigation of the Reaction of Boron Monoxide (BO; $X^2\Sigma^+$) with 1,3-Butadiene ($\text{CH}_2\text{CHCHCH}_2$; X^1A_g) and Its Deuterated Counterparts**
Surajit Maity, Beni B. Dangi, Dorian S. N. Parker, Ralf. I. Kaiser, Hong-Mao Lin, Hai-Ping E, Bing-Jian Sun, and A. H. H. Chang
The Journal of Physical Chemistry A 2015 119 (7), 1094-1107
DOI: 10.1021/jp511715e
- 3. Binding Strength of Porphyrin–Gold Nanoparticle Hybrids Based on Number and Type of Linker Moieties and a Simple Method To Calculate Inner Filter Effects of Gold Nanoparticles Using Fluorescence Spectroscopy**
Ahson J. Shaikh, Faiz Rabbani, Tauqir A. Sherazi, Zafar Iqbal, Sadullah Mir, and Sohail A. Shahzad
The Journal of Physical Chemistry A 2015 119 (7), 1108-1116
DOI: 10.1021/jp510924n
- 4. Acid–Base Formalism in Dispersion-Stabilized S–H \cdots Y (Y=O, S) Hydrogen-Bonding Interactions**
Aditi Bhattacharjee, Yoshiyuki Matsuda, Asuka Fujii, and Sanjay Wategaonkar
The Journal of Physical Chemistry A 2015 119 (7), 1117-1126
DOI: 10.1021/jp511904a
- 5. Dissociative Photoionization of Quinoline and Isoquinoline**
Jordy Bouwman, Bálint Sztáray, Jos Oomens, Patrick Hemberger, and Andras Bodi
The Journal of Physical Chemistry A 2015 119 (7), 1127-1136
DOI: 10.1021/jp5121993
- 6. Infrared Photoisomerization of 1-Propanol CD₃ and OD Trapped in Four Cryogenic Matrices: Ne, N₂, Ar, and Xe**
J. A. Noble and S. Coussan
The Journal of Physical Chemistry A 2015 119 (7), 1137-1145
DOI: 10.1021/jp5126359
- 7. Vibrationally Resolved Photoelectron Spectroscopy of Electronic Excited States of DNA Bases: Application to the \tilde{A} State of Thymine Cation**
Majdi Hochlaf, Yi Pan, Kai-Chung Lau, Youssef Majdi, Lionel Poisson, Gustavo A. Garcia, Laurent Nahon, Muneerah Mogren Al Mogren, and Martin Schwell
The Journal of Physical Chemistry A 2015 119 (7), 1146-1153
DOI: 10.1021/acs.jpca.5b00466
- 8. Changes to the Chemical Composition of Soot from Heterogeneous Oxidation Reactions**
Eleanor C. Browne, Jonathan P. Franklin, Manjula R. Canagaratna, Paola Massoli, Thomas W. Kirchstetter, Douglas R. Worsnop, Kevin R. Wilson, and Jesse H. Kroll
The Journal of Physical Chemistry A 2015 119 (7), 1154-1163

DOI: 10.1021/jp511507d

9. Theoretical and Thermochemical Network Approaches To Determine the Heats of Formation for HO₂ and Its Ionic Counterparts

Ádám Ganyecz, József Csontos, Balázs Nagy, and Mihály Kállay

The Journal of Physical Chemistry A **2015** *119* (7), 1164-1176

DOI: 10.1021/jp5104643

10. Homoleptic Tetranuclear Rhodium Carbonyls: Comparison with Their Iridium Analogues

Shida Gong, Qiong Luo, Na Dou, Qingkui Chi, Bin Peng, Yaoming Xie, R. Bruce King, and Henry F. Schaefer, III

The Journal of Physical Chemistry A **2015** *119* (7), 1177-1189

DOI: 10.1021/jp511016v

11. Toward Selection of Efficient Density Functionals for van der Waals Molecular Complexes: Comparative Study of C–H⋯π and N–H⋯π Interactions

Guvanchmyrat Paytakov, Tandabany Dinadayalane, and Jerzy Leszczynski

The Journal of Physical Chemistry A **2015** *119* (7), 1190-1200

DOI: 10.1021/jp511450u

12. Aromatic Pathways in Carbothiaporphyrins

Rashid R. Valiev, Heike Fliegl, and Dage Sundholm

The Journal of Physical Chemistry A **2015** *119* (7), 1201-1207

DOI: 10.1021/jp5120652

13. Application of the Unified Singlet and Triplet Electron-Pair Extrapolation Scheme with Basis Set Rehierarchization to Tensorial Properties

F. N. N. Pansini, A. C. Neto, and A. J. C. Varandas

The Journal of Physical Chemistry A **2015** *119* (7), 1208-1217

DOI: 10.1021/jp512397n

14. Effect of Capping Ligands and TiO₂ Supporting on the Optical Properties of a (CdSe)₁₃ Cluster

Roger Nadler and Javier Fernandez Sanz

The Journal of Physical Chemistry A **2015** *119* (7), 1218-1227

DOI: 10.1021/acs.jpca.5b00625