

TU  
J80/pol

SEPTEMBER 18, 2014

VOLUME 118

NUMBER 37

[pubs.acs.org/JPCA](http://pubs.acs.org/JPCA)

# THE JOURNAL OF PHYSICAL CHEMISTRY A

**Castleman Research Group Interests  
(see page 5A)**

**Superatoms**

Atoms: Cl (18-e<sup>-</sup>) has 3d<sup>0</sup>, 3p<sup>5</sup>, 3s<sup>2</sup>, 2p<sup>5</sup>, 2s<sup>2</sup>, 1s<sup>2</sup>. Clusters: Al<sub>13</sub> (40-e<sup>-</sup>) has 2p<sup>6</sup>, 1f<sup>14</sup>, 2s<sup>2</sup>, 1d<sup>10</sup>, 1p<sup>6</sup>, 1s<sup>2</sup> (20-e<sup>-</sup>).

Mass spectra show Intensity (Arb. Units) vs M/E. Low oxygen: Al<sub>7</sub><sup>+</sup> at ~150, Al<sub>13</sub><sup>+</sup> at ~330, Al<sub>15</sub><sup>+</sup> at ~600. High oxygen: Al<sub>7</sub><sup>+</sup> at ~150, Al<sub>13</sub><sup>+</sup> at ~330, Al<sub>15</sub><sup>+</sup> at ~600.

**Velocity Map Imaging**

Intensity vs Electron binding energy (eV). Top: Ni<sup>+</sup> shows a sharp peak at ~0.8 eV. Bottom: TiO<sup>+</sup> shows a sharp peak at ~0.8 eV and a smaller peak at ~1.2 eV.

**Met-Cars**

A complex polyhedral cluster composed of many small spheres connected by a network of lines.

**Coulomb Explosion**

Volts vs Microseconds. Peak at ~6.55 V is labeled "Forward ejected ions that pass through the reflectron". Peak at ~6.6 V is labeled "Backward ejected ions that collide with TOF-I". A blue shaded area is labeled "Undetected".

**Catalysis**

Reaction scheme: V<sub>2</sub>O<sub>5</sub> + C<sub>2</sub>H<sub>4</sub> → V<sub>2</sub>O<sub>5</sub><sup>+</sup> + C<sub>2</sub>H<sub>4</sub><sup>+</sup> (Defect Site - Missing V). Step Edges are also shown. Products: VO<sub>2</sub><sup>+</sup> + C<sub>4</sub>H<sub>10</sub>, V<sub>2</sub>O<sub>4</sub><sup>+</sup> + CH<sub>2</sub>F<sub>2</sub>.

**Ion Molecule Reactions**

Ion Intensity (arb. units) vs Mass (m/z). Peaks are labeled: C<sub>2</sub>H<sub>5</sub><sup>+</sup>, V<sub>2</sub>O<sub>5</sub><sup>+</sup>, V<sub>2</sub>O<sub>4</sub><sup>+</sup>, V<sub>2</sub>O<sub>3</sub>H<sup>+</sup>, V<sub>2</sub>O<sub>2</sub>C<sub>2</sub>H<sub>6</sub><sup>+</sup>, and V<sub>2</sub>O<sub>2</sub>.

**A. W. CASTLEMAN, JR. FESTSCHRIFT**



**ACS Publications**  
Most Trusted. Most Cited. Most Read.

[www.acs.org](http://www.acs.org)

SEPTEMBER 18, 2014

VOLUME 118 ISSUE 37

JPCAFH 118(37) 8011–8624 (2014)

ISSN 1089-5639

Registered in the U.S. Patent and Trademark Office

© 2014 by the American Chemical Society

**ON THE COVER:** Examples of Will's research interests, which exemplify some of his significant contributions to the field of cluster science and physical chemistry. (Top left) Electronic configurations and experimental evidence of superatom clusters. (Top center) Photoelectron velocity map images obtained from atoms and molecules (adapted from Castleman, A. W., Jr. From Elements to Clusters: The Periodic Table Revisited. *J. Phys. Chem. Lett.* 2011, 2, 1062–1069). (Top right) Structural model of metallocarbohedrene (Met-Car) clusters. (Bottom right) Coulomb explosion as a mechanistic probe of femtosecond cluster dynamics. (Bottom center) Mass spectrometric analysis of ion–molecule reactions in a cluster model system. (Bottom left) Clusters as model catalysts [Zemski, K. A.; Justes, D. R.; Castleman, A. W., Jr. Studies of Metal Oxide Clusters: Elucidating Reactive Sites Responsible for the Activity of Transition Metal Oxide Catalysts. *J. Phys. Chem. B*, 2002, 106, 6136–6148 (cover art)]. (Center) Images of femtosecond and gas-phase instruments utilized by the Castleman research group. This special issue was organized by Guest Editors Mostafa A. El-Sayed, Grant E. Johnson, and Kenneth L. Knappenberger, Jr.

## SPECIAL ISSUE: A. W. CASTLEMAN, JR. FESTSCHRIFT

Guest Editors: Mostafa A. El-Sayed, Grant E. Johnson, and Kenneth L. Knappenberger, Jr.

### Special Issue Preface

8011

[dx.doi.org/10.1021/jp501364m](http://dx.doi.org/10.1021/jp501364m)

Tribute to A. W. Castleman, Jr.

Kenneth L. Knappenberger Jr.,\* Grant E. Johnson, and Mostafa A. El-Sayed

8014

[dx.doi.org/10.1021/jp501365v](http://dx.doi.org/10.1021/jp501365v)

Autobiography of A. W. Castleman, Jr.

8019 Honors and Awards from the Presidents of C-20, U-MRS, and OH-Electrode.

[dx.doi.org/10.1021/jp505726z](http://dx.doi.org/10.1021/jp505726z)

Honors and Awards of A. W. Castleman, Jr.

8020

[dx.doi.org/10.1021/jp501370v](http://dx.doi.org/10.1021/jp501370v)

Colleagues of A. W. Castleman, Jr.

8021

[dx.doi.org/10.1021/jp501366z](http://dx.doi.org/10.1021/jp501366z)

Curriculum Vitae of A. W. Castleman, Jr.

8025

[dx.doi.org/10.1021/jp5013686](http://dx.doi.org/10.1021/jp5013686)

Publications of A. W. Castleman, Jr.

# Articles

8050

[dx.doi.org/10.1021/jp406540p](https://doi.org/10.1021/jp406540p)**On the Size and Structure of Helium Snowballs Formed around Charged Atoms and Clusters of Noble Gases**

Peter Barth, Christian Leidlmair, Stephan Denifl, Paul Scheier,\* and Olof Echt\*

8060

[dx.doi.org/10.1021/jp407698a](https://doi.org/10.1021/jp407698a)**The  $\alpha$ -Effect in Gas-Phase  $S_N2$  Reactions of Microsolvated Anions: Methanol as a Solvent**

Ditte L. Thomsen, Jennifer N. Reece, Charles M. Nichols, Steen Hammerum, and Veronica M. Bierbaum\*

8067

[dx.doi.org/10.1021/jp408147f](https://doi.org/10.1021/jp408147f)**Dynamics of Thermal Electron Emission from Highly Excited  $C_{60}$** 

J. Olof Johansson, Gordon G. Henderson, and Eleanor E. B. Campbell\*

8074

S

[dx.doi.org/10.1021/jp410009a](https://doi.org/10.1021/jp410009a)**Covalently Bound Tetracoordinated Organoborons as Superhalogens: A Combined Negative Ion Photoelectron Spectroscopy and Theoretical Study**

Jian Zhang, Ping Yang,\* Zhen-Rong Sun,\* and Xue-Bin Wang\*

8081

[dx.doi.org/10.1021/jp4108624](https://doi.org/10.1021/jp4108624)**Investigation of Carbon Buildup in Simulations of Multi-Impact Bombardment of Si with 20 keV  $C_{60}$  Projectiles**

Kristin D. Krantzman,\* Clarissa A. Briner, and Barbara J. Garrison

8088

S

[dx.doi.org/10.1021/jp4116172](https://doi.org/10.1021/jp4116172)**Akali Metal Cation Interactions with 15-Crown-5 in the Gas Phase: Revisited**

P. B. Armentrout,\* C. A. Austin, and M. T. Rodgers\*

8098

S

[dx.doi.org/10.1021/jp411867q](https://doi.org/10.1021/jp411867q)**Complexes between Planar Boron Clusters and Transition Metals: A Photoelectron Spectroscopy and Ab Initio Study of  $CoB_{12}^-$  and  $RhB_{12}^-$** 

Ivan A. Popov, Wei-Li Li, Zachary A. Piazza, Alexander I. Boldyrev,\* and Lai-Sheng Wang\*

8106

S

[dx.doi.org/10.1021/jp411961q](https://doi.org/10.1021/jp411961q)**Consecutive Oxygen-for-Sulfur Exchange Reactions between Vanadium Oxide Cluster Anions and Hydrogen Sulfide**

Mei-Ye Jia, Bo Xu, Ke Deng, Sheng-Gui He,\* and Mao-Fa Ge\*

8115

[dx.doi.org/10.1021/jp412360b](https://doi.org/10.1021/jp412360b)**Electronic and Vibrational Properties of *meso*-Tetraphenylporphyrin on Silver Substrates**

Patrick Z. El-Khoury, Karoliina Honkala, and Wayne P. Hess\*

**Size-Focusing Synthesis of Gold Nanoclusters with *p*-Mercaptobenzoic Acid**

Laura M. Tvedte and Christopher J. Ackerson\*

**Influence of the d Orbital Occupation on the Structures and Sequential Binding Energies of Pyridine to the Late First-Row Divalent Transition Metal Cations: A DFT Study**

Holliness Nose and M. T. Rodgers\*

**Temperature-Dependent Kinetics of Charge Transfer, Hydrogen-Atom Transfer, and Hydrogen-Atom Expulsion in the Reaction of CO<sup>+</sup> with CH<sub>4</sub> and CD<sub>4</sub>**

Joshua J. Melko, Shaun G. Ard, Ryan S. Johnson, Nicholas S. Shuman, Hua Guo, and Albert A. Viggiano\*

**Alkyl Nitrate Formation from the Reactions of C<sub>8</sub>–C<sub>14</sub> *n*-Alkanes with OH Radicals in the Presence of NO<sub>x</sub>: Measured Yields with Essential Corrections for Gas–Wall Partitioning**

Geoffrey K. Yeh and Paul J. Ziemann\*

**Alanate Anion, AlH<sub>4</sub><sup>−</sup>: Photoelectron Spectrum and Computations**

J. D. Graham, A. M. Buytendyk, X. Zhang, E. L. Collins, B. Kiran, G. Ganterfoer, B. W. Eichhorn, G. L. Gutsev,\* S. Behera, P. Jena,\* and K. H. Bowen\*

**Oxygen–Sulfur Exchange and the Gas-Phase Reactivity of Cobalt Sulfide Cluster Anions with Molecular Oxygen**

Mei-Ye Jia, Zhixun Luo,\* Sheng-Gui He,\* and Mao-Fa Ge

**Controlling Dissociation of Alkyl Phenyl Ketone Radical Cations in the Strong-Field Regime through Hydroxyl Substitution Position**

Katharine Moore Tibbetts, Timothy Bohinski, Kristin Munkerup, Maryam Tarazkar, and Robert Levis\*

**Experimental Study of the Competitive Adsorption of HNO<sub>3</sub> and H<sub>2</sub>O on Surfaces by Using Brewster Angle Cavity Ring-Down Spectroscopy in the 295–345 nm Region**

Juan Du, Robert G. Keesee,\* and Lei Zhu\*

**Enhanced Immobilization of Gold Nanoclusters on Graphite**

P. Rodríguez-Zamora, F. Yin, and R. E. Palmer\*

8188

S

[dx.doi.org/10.1021/jp500964j](https://doi.org/10.1021/jp500964j)**Vibrational Spectroscopy of the Water–Nitrate Complex in the O–H Stretching Region**

Nadja Heine, Eric G. Kratz, Rishu Bergmann, Daniel P. Schofield, Knut R. Asmis,\* Kenneth D. Jordan,\* and Anne B. McCoy

8198

S

[dx.doi.org/10.1021/jp500928t](https://doi.org/10.1021/jp500928t)**Structure Assignment, Electronic Properties, and Magnetism Quenching of Endohedrally Doped Neutral Silicon Clusters,  $\text{Si}_n\text{Co}$  ( $n = 10–12$ )**

Yejun Li, Nguyen Minh Tam, Pieterjan Claes, Alex P. Woodham, Jonathan T. Lyon, Vu Thi Ngan, Minh Tho Nguyen, Peter Lievens,\* André Fielicke, and Ewald Janssens

8204

S

[dx.doi.org/10.1021/jp501002x](https://doi.org/10.1021/jp501002x)**Theoretical Investigation of Water Oxidation Processes on Small  $\text{Mn}_x\text{Ti}_{2-x}\text{O}_4$  ( $x = 0–2$ ) Complexes**

Choongkeun Lee and Christine M. Aikens\*

8222

S

[dx.doi.org/10.1021/jp501015k](https://doi.org/10.1021/jp501015k)**Systematic Analysis of Reactivities and Fragmentation of Glutathione and Its Isomer GluCysGly**

Shan Feng, Xiaoyan Zheng, Dong Wang, Yiyi Gong, Qingtao Wang, and Haiteng Deng\*

8229

S

[dx.doi.org/10.1021/jp5010192](https://doi.org/10.1021/jp5010192)**Sensitivity and Selectivity of Switchable Reagent Ion Soft Chemical Ionization Mass Spectrometry for the Detection of Picric Acid**

Bishu Agarwal, Ramón González-Méndez, Matteo Lanza, Philipp Sulzer, Tilmann D. Märk, Neil Thomas, and Chris A. Mayhew\*

8237

S

[dx.doi.org/10.1021/jp501046r](https://doi.org/10.1021/jp501046r)**Wetting Transitions of Water on Graphite and Graphene**

Hye-Young Kim,\* Maria Cristina dos Santos, and Milton W. Cole

8242

S

[dx.doi.org/10.1021/jp501038z](https://doi.org/10.1021/jp501038z)**Desorption Kinetics of Methanol, Ethanol, and Water from Graphene**

R. Scott Smith,\* Jesper Matthiesen, and Bruce D. Kay\*

8251

S

[dx.doi.org/10.1021/jp5010488](https://doi.org/10.1021/jp5010488)**Formation of Covalently Bonded Polycyclic Hydrocarbon Ions by Intracluster Polymerization of Ionized Ethynylbenzene Clusters**

Paul O. Momoh, Isaac K. Attah, M. Samy El-Shall,\* René P. F. Kinters, John M. Pinski, and Samuel A. Abrash

8264

S

[dx.doi.org/10.1021/jp501073a](https://doi.org/10.1021/jp501073a)**Cyclopentanethiolato-Protected  $\text{Au}_{36}(\text{SC}_5\text{H}_9)_{24}$  Nanocluster: Crystal Structure and Implications for the Steric and Electronic Effects of Ligand**

Anindita Das, Chong Liu, Chenjie Zeng, Gao Li, Tao Li, Nathaniel L. Rosi, and Rongchao Jin\*

8270

[dx.doi.org/10.1021/jp5010902](https://doi.org/10.1021/jp5010902)**Photoelectron Imaging Spectroscopy of the Small Sodium Cluster Anions  $\text{Na}_3^-$ ,  $\text{Na}_5^-$ , and  $\text{Na}_7^-$** 

Christof Bartels,\* Christian Hock, Raphael Kuhnen, and Bernd v. Issendorff

8277

[dx.doi.org/10.1021/jp501059c](https://doi.org/10.1021/jp501059c)**Studies of Structural Isomers *o*-, *m*-, and *p*-Fluorophenylacetylene by Two-Color Resonant Two-Photon Mass-Analyzed Threshold Ionization Spectroscopy**

Vidya S. Shrivastava, Aniket Kundu, G. Naresh Patwari, and Wen Bih Tzeng\*

8287

[dx.doi.org/10.1021/jp502063e](https://doi.org/10.1021/jp502063e)**Interactions of Cytochrome c with N-Acylated Phosphatidylethanolamine Lipids**

Emily S. Mohn, Jung-Min Lee, Christopher Beaver, Gerri Tobbe, Sean M. McCarthy, Edward O'Neil, Bradley D. Smith, and John J. Breen\*

8293

[dx.doi.org/10.1021/jp501111f](https://doi.org/10.1021/jp501111f)**Water-Induced Adsorption of Carbon Monoxide and Oxygen on the Gold Dimer Cation**

Tomonori Ito, G. Naresh Patwari, Masashi Arakawa, and Akira Terasaki\*

8298

[dx.doi.org/10.1021/jp5011007](https://doi.org/10.1021/jp5011007)**Formation and Electronic Structures of Organoeuropium Sandwich Nanowires**

Natsuki Hosoya, Ryuta Takegami, Jun-ichi Suzumura, Keizo Yada, Ken Miyajima, Masaaki Mitsui, Mark B. Knickelbein, Satoshi Yabushita, and Atsushi Nakajima\*

8309

[dx.doi.org/10.1021/jp5011378](https://doi.org/10.1021/jp5011378)**Catalytic Oxidation of Methanol to Formaldehyde by Mass-Selected Vanadium Oxide Clusters Supported on a  $\text{TiO}_2(110)$  Surface**

Scott P. Price, Xiao Tong, Claron Ridge, Hunter L. Neilson, Joshua W. Buffon, Jeremy Robins, Horia Metiu, Michael T. Bowers, and Steven K. Buratto\*

8314

[dx.doi.org/10.1021/jp501124q](https://doi.org/10.1021/jp501124q)**Isolation and Structural Characterization of a Silver–Platinum Nanocluster,  $\text{Ag}_4\text{Pt}_2(\text{DMSA})_4$** 

Scott R. Bilek, Ayusman Sen,\* Anthony F. Pedicini, Arthur C. Reber, and Shiv N. Khanna\*

8320

[dx.doi.org/10.1021/jp501143u](https://doi.org/10.1021/jp501143u)**Excited State Electronic Structures of 5,10-Methenyltetrahydrofolate and 5,10-Methylenetetrahydrofolate Determined by Stark Spectroscopy**

Raymond F. Pauszek III, Goutham Kodali, and Robert J. Stanley\*

8329

[dx.doi.org/10.1021/jp501123y](https://doi.org/10.1021/jp501123y)**Metallic Copper Colloids by Reductive Laser Ablation of Nonmetallic Copper Precursor Suspensions**

Christian A. Schaumberg, Markus Wollgarten, and Klaus Rademann\*

Spectroscopy of Homo- and Heterodimers of Silver and Gold Nanocubes as a Function of Separation: A DDA Simulation  
Nasrin Hooshmand, Daniel O'Neil, Abdullah M. Asiri, and Mostafa El-Sayed\*

Reactivity of Silver Clusters Anions with Ethanethiol

Zhixun Luo,\* Gabriel U. Gamboa, Meiyue Jia, Arthur C. Reber, Shiv N. Khanna,\* and A. W. Castleman Jr.\*

Superatomic S<sup>2</sup> Silver Clusters Stabilized by a Thiolate–Phosphine Monolayer: Insight into Electronic and Optical Properties of Ag<sub>14</sub>(SC<sub>6</sub>H<sub>5</sub>F<sub>2</sub>)<sub>12</sub>(PPh<sub>3</sub>)<sub>8</sub> and Ag<sub>16</sub>(SC<sub>6</sub>H<sub>5</sub>F<sub>2</sub>)<sub>14</sub>(DPPE)<sub>4</sub>

Lars Gell, Lauri Lehtovaara, and Hannu Häkkinen\*

Gas-Phase Synthesis and Structure of Wade-Type Ruthenium Carbonyl and Hydrido Carbonyl Clusters

Sandra M. Lang, Sandra U. Förtig, Thorsten M. Bernhardt,\* Marjan Krstić, and Vlasta Bonačić-Koutecký\*

Effects of Translational and Vibrational Excitation on the Reaction of HOD<sup>+</sup> with C<sub>2</sub>H<sub>2</sub> and C<sub>2</sub>D<sub>2</sub>: Mode- and Bond-Specific Effects in Exoergic Proton Transfer

David M. Bell, Collin R. Howder, and Scott L. Anderson\*

One- and Two-Color Resonant Photoionization Spectroscopy of Chromium-Doped Helium Nanodroplets

Markus Koch,\* Andreas Kautsch, Florian Lackner, and Wolfgang E. Ernst\*

Hydrogen Bonding Constrains Free Radical Reaction Dynamics at Serine and Threonine Residues in Peptides

Daniel A. Thomas, Chang Ho Sohn, Jinshan Gao, and J. L. Beauchamp\*

Chiral Nanostructures Studied Using Polarization-Dependent NOLES Imaging

Jeremy W. Jarrett, Patrick J. Herbert, Scott Dhuey, Adam M. Schwartzberg, and Kenneth L. Knappenberger Jr.\*

Experiment and Theory Elucidate the Multichannel Predissociation Dynamics of the HCl Trimer: Breaking Up Is Hard To Do

John S. Mancini, Amit K. Samanta, Joel M. Bowman,\* and Hanna Reisler\*

**Vibrating  $H_2^+({}^2\Sigma_g^+, JM = 00)$  Ion as a Pulsating Quantum Bubble in the Laboratory Frame**  
Jörn Manz,\* Jhon Fredy Pérez-Torres, and Yonggang Yang

**Validation of Classical Force Fields for the Description of Thermo-Mechanical Properties of Transition Metal Materials**  
Gennady B. Sushko, Alexey V. Verkhovtsev, and Andrey V. Solov'yov\*

**Exploring Ultrafast Dynamics of Pyrazine by Time-Resolved Photoelectron Imaging**  
Gaia Tomasello, Alexander Humeniuk, and Roland Mitrč\*

**Promotional Effects of Mesoporous Zeolites with Pt Nanoparticle Catalysts during Reforming of Methylcyclopentane**  
Kyungsu Na, Nathan Musselwhite, Xiaojun Cai, Selim Alayoglu,\* and Gabor A. Somorjai\*

**Ion Mobility Spectrometry, Infrared Dissociation Spectroscopy, and ab Initio Computations toward Structural Characterization of the Deprotonated Leucine-Enkephalin Peptide Anion in the Gas Phase**

Florian Schinle, Christoph R. Jacob,\* Arron B. Wolk, Jean-François Greisch, Matthias Vonderach, Patrick Weis, Oliver Hampe, Mark A. Johnson,\* and Manfred M. Kappes\*

**Investigating the Synthesis of Ligated Metal Clusters in Solution Using a Flow Reactor and Electrospray Ionization Mass Spectrometry**

Astrid Olivares, Julia Laskin, and Grant E. Johnson\*

**Receptor–Ligand Interaction at 5-HT<sub>3</sub> Serotonin Receptors: A Cluster Approach**

Bijan K. Rao, Devleena Samanta, Shawn Joshi, Kinjal Basu, Sheryl D. Baldwin, Amrita Jha, Małgorzata Dukat, Richard A. Glennon, and Puru Jena\*

**Size- and Support-Dependent Evolution of the Oxidation State and Structure by Oxidation of Subnanometer Cobalt Clusters**

Chunrong Yin, Fan Zheng, Sungsik Lee, Jinghua Guo, Wei-Cheng Wang, Gihan Kwon, Viktor Vajda, Hsien-Hau Wang, Byeongdu Lee, Janae DeBartolo, Sönke Seifert, Randall E. Winans, and Stefan Vajda\*

**Boron Substitution in Aluminum Cluster Anions: Magic Clusters and Reactivity with Oxygen**

Jordan C. Smith, Arthur C. Reber, Shiv N. Khanna, and A. W. Castleman Jr.\*

8493

dx.doi.org/10.1021/jp502021k

**RH and H<sub>2</sub> Production in Reactions between ROH and Small Molybdenum Oxide Cluster Anions**

Sarah E. Waller and Caroline C. Jarrold\*

8505

dx.doi.org/10.1021/jp502186q

**Photochemical Kinetics of Pyruvic Acid in Aqueous Solution**

Allison E. Reed Harris, Barbara Ervens, Richard K. Shoemaker, Jay A. Kroll, Rebecca J. Rapf, Elizabeth C. Griffith, Anne Monod, and Veronica Vaida\*

8517

dx.doi.org/10.1021/jp502238c

**Time-Resolved Excited State Energetics of the Solvated Electron in Sodium-Doped Water Clusters**

J. P. Müller, N. Zhavoronkov, I. V. Hertel, and C. P. Schulz\*

8525

dx.doi.org/10.1021/jp5022642

**Experimental Binding Energies for the Metal Complexes [Mg(NH<sub>3</sub>)<sub>n</sub>]<sup>2+</sup>, [Ca(NH<sub>3</sub>)<sub>n</sub>]<sup>2+</sup>, and [Sr(NH<sub>3</sub>)<sub>n</sub>]<sup>2+</sup> for n = 4–20 Determined from Kinetic Energy Release Measurements**

E. Bruzzi, G. Raggi, R. Parajuli, and A. J. Stace\*

8533

dx.doi.org/10.1021/jp5024229

**Heterogeneously Substituted Radicals and Carbenes: Photoelectron Imaging of the FC(H)CN<sup>-</sup> and FCCN<sup>-</sup> Anions**

Andrew R. Dixon, Dmitry Khuseynov, and Andrei Sanov\*

8542

dx.doi.org/10.1021/jp5024247

**Formation of Neutral In<sub>m</sub>C<sub>n</sub> Clusters under C<sub>60</sub> Ion Bombardment of Indium**

Lars Breuer, Andrew Kucher, Matthias Herder, Andreas Wucher, and Nicholas Winograd\*

8553

dx.doi.org/10.1021/jp502459r

**Molecular Dynamics Simulations and Electronic Excited State Properties of a Self-Assembled Peptide Amphiphile Nanofiber with Metalloporphyrin Arrays**

Tao Yu, One-Sun Lee, and George C. Schatz\*

8563

dx.doi.org/10.1021/jp502540n

**Identification of Phase Boundaries in Surfactant Solutions via Compton Spectrum Quenching**

Denis E. Bergeron\*

8572

dx.doi.org/10.1021/jp502736p

**Size-Dependent Self-Limiting Oxidation of Free Palladium Clusters**

Sandra M. Lang, Irene Fleischer, Thorsten M. Bernhardt,\* Robert N. Barnett, and Uzi Landman\*

**Binding Water Clusters to an Aromatic-Rich Hydrophobic Pocket: [2.2.2]Paracyclophane-(H<sub>2</sub>O)<sub>n</sub>, n = 1–5**  
Evan G. Buchanan and Timothy S. Zwier\*

**Structure and Stability of Phenoxide and Fluorophenoxide Anions Investigated with Infrared Multiple-Photon Dissociation and Detachment Spectroscopy and Tandem Mass Spectrometry**

Jeffrey D. Steill, Amanda L. May, Shawn R. Campagna, Jos Oomens, and Robert N. Compton\*

**Pathways to Soot Oxidation: Reaction of OH with Phenanthrene Radicals**

David E. Edwards, Dmitry Yu. Zubarev, William A. Lester Jr., and Michael Frenklach\*

**Exposing the Role of Electron Correlation in Strong-Field Double Ionization: X-ray Transient Absorption of Orbital Alignment in Xe<sup>+</sup> and Xe<sup>2+</sup>**

Scott G. Sayres, Erik R. Hosler, and Stephen R. Leone\*