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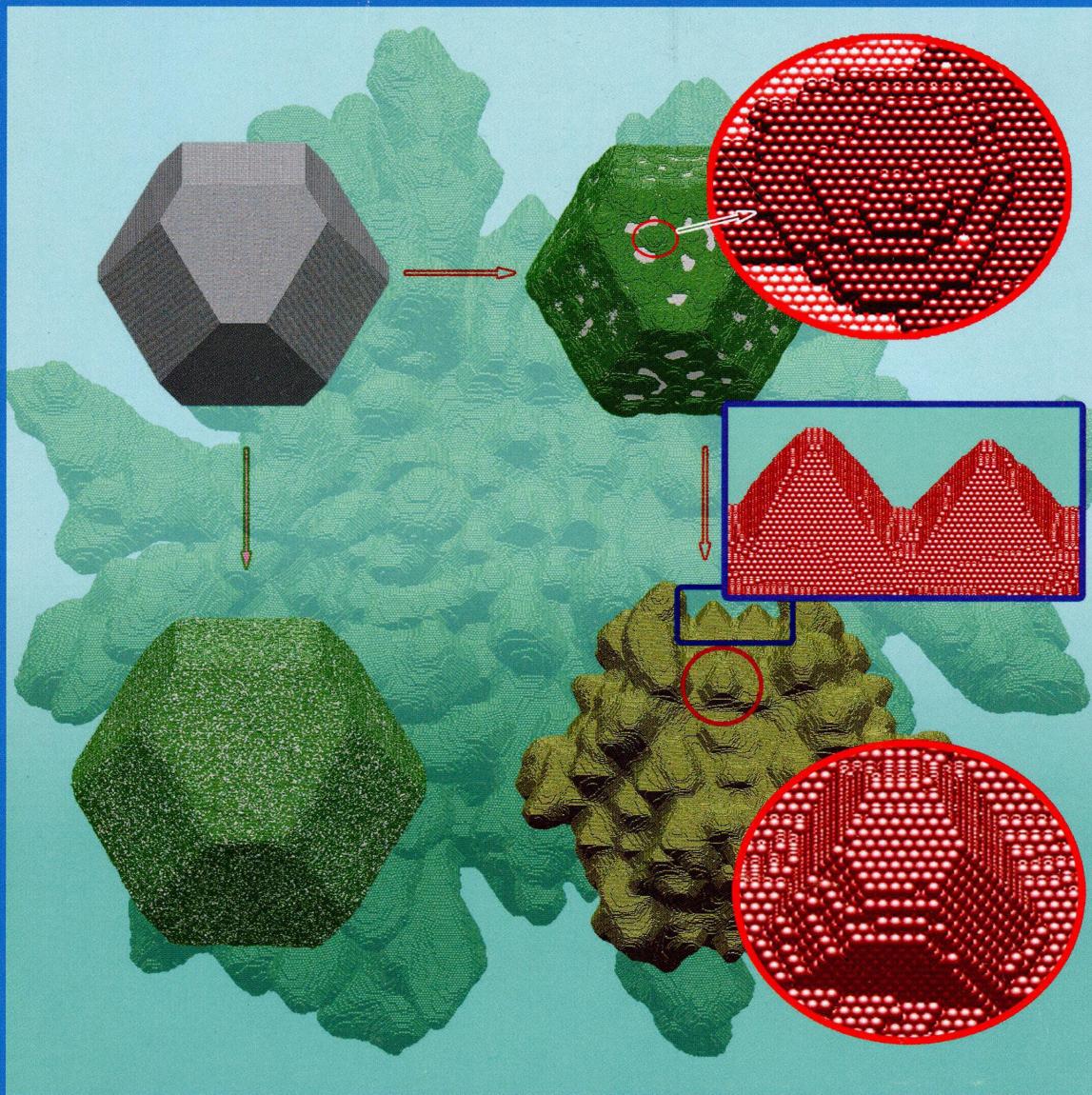
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# THE JOURNAL OF PHYSICAL CHEMISTRY C

Kinetic Modeling of  
Shell Growth and  
Morphology of  
Core–Shell  
Noble-Metal  
Nanoparticles  
(see page 24959)



ENERGY CONVERSION AND STORAGE, OPTICAL AND ELECTRONIC DEVICES,  
INTERFACES, NANOMATERIALS, AND HARD MATTER

**ON THE COVER:** Kinetic modeling of shell growth and morphology of core–shell noble-metal nanoparticles. The kinetic Monte Carlo modeling approach is shown to reproduce smooth-shell and cluster-structured shell growth morphologies identified in recent experiments on core–shell noble-metal nanoparticle synthesis, including the formation of smooth epitaxially grown shells. The effects of temperature and supply of matter on the resulting shell morphology are considered for growth on presynthesized nanocrystal cores. See page 24959.

## Articles

### Energy Conversion and Storage; Energy and Charge Transport

24811 dx.doi.org/10.1021/jp502650u

#### Electrical Properties of Self-Assembled Films of Polyaniline/Carbon Nanotubes Composites

Luiz C. Mariano, Rodrigo V. Salvatierra, Carlos E. Cava, Marlus Koehler, Aldo J. G. Zarbin, and Lucimara S. Roman\*

24819 dx.doi.org/10.1021/jp505463v

#### Graphene-Induced Enhancement of n-Type Mobility in Perylenediimide Thin Films

Srinivasa Rao Pathipati, Egon Pavlica, Andrea Schlierf, Mirella El Gemayel, Paolo Samori, Vincenzo Palermo, and Gvido Bratina\*

24827 dx.doi.org/10.1021/jp5073044

#### Energy States of Ligand Capped Ag Nanoparticles: Relating Surface Plasmon Resonance to Work Function

Anup L. Dadlani, Peter Schindler, Manca Logar, Steve P. Walch, and Fritz B. Prinz\*

24833 dx.doi.org/10.1021/jp507372n

#### Carbon Nitride Photocatalysts for Water Splitting: A Computational Perspective

Cristina Butchosa, Pierre Guiglion, and Martijn A. Zwijnenburg\*

24843 dx.doi.org/10.1021/jp507430x

#### Radiative Recombination and Photoconversion of Methylammonium Lead Iodide Perovskite by First Principles: Properties of an Inorganic Semiconductor within a Hybrid Body

Alessio Filippetti,\* Pietro Delugas, and Alessandro Mattoni\*

24854 dx.doi.org/10.1021/jp507435a

#### Exciton Level Structure and Dynamics in Tubular Porphyrin Aggregates

Yan Wan, Anna Stradomska, Sarah Fong, Zhi Guo, Richard D. Schaller, Gary P. Wiederrecht, Jasper Knoester,\* and Libai Huang\*

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[dx.doi.org/10.1021/jp5075779](https://doi.org/10.1021/jp5075779)

**Highly Oxidized Graphene Anchored Ni(OH)<sub>2</sub> Nanoflakes as Pseudocapacitor Materials for Ultrahigh Loading Electrode with High Areal Specific Capacitance**

Yongfu Tang,\* Yanyan Liu, Wanchun Guo, Teng Chen, Hongchao Wang, Shengxue Yu, and Faming Gao

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[dx.doi.org/10.1021/jp508814y](https://doi.org/10.1021/jp508814y)

**Self-Assembled CoS<sub>2</sub> Nanocrystal Film as an Efficient Counter Electrode for Dye-Sensitized Solar Cells**

Jiarui Jin, Xuehua Zhang,\* and Tao He\*

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[dx.doi.org/10.1021/jp508840s](https://doi.org/10.1021/jp508840s)

**Cation Disorder Regulation by Microstate Configurational Entropy in Photovoltaic Absorber Materials Cu<sub>2</sub>ZnSn(S,Se)<sub>4</sub>**

ShunLi Shang,\* Yi Wang, Greta Lindwall, Neal R. Kelly, Tim J. Anderson, and Zi-Kui Liu

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[dx.doi.org/10.1021/jp508933c](https://doi.org/10.1021/jp508933c)

**Facile and Green Preparation for the Formation of MoO<sub>2</sub>-GO Composites as Anode Material for Lithium-Ion Batteries**

Shan Hu, Fei Yin, Evan Uchaker, Wen Chen,\* Ming Zhang, Jing Zhou, Yanyuan Qi, and Guozhong Cao\*

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Chi-Yuan Lin, Hung-Wei Shiu, Lo-Yueh Chang, Chia-Hao Chen, Chen-Shiung Chang, and Forest Shih-Sen Chien\*

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**Photocatalytic Activity of TiO<sub>2</sub> Modified with Hexafluorometallates—Fine Tuning of Redox Properties by Redox-Innocent Anions**

Marta Buchalska,\* Michał Pacia, Marcin Kobielsz, Marcin Surówka, Elżbieta Świątek, Ewelina Właźlik, Konrad Szaciłowski,\* and Wojciech Macyk\*

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[dx.doi.org/10.1021/jp507142v](https://doi.org/10.1021/jp507142v)

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[dx.doi.org/10.1021/jp505696m](https://doi.org/10.1021/jp505696m)**Confinement Effect of Zeolite Cavities on Methanol-to-Olefin Conversion: A Density Functional Theory Study**

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[dx.doi.org/10.1021/jp505770t](https://doi.org/10.1021/jp505770t)**Surface Electric Fields of Aqueous Solutions of  $\text{NH}_4\text{NO}_3$ ,  $\text{Mg}(\text{NO}_3)_2$ ,  $\text{NaNO}_3$ , and  $\text{LiNO}_3$ : Implications for Atmospheric Aerosol Chemistry**

Wei Hua, Dominique Verreault, and Heather C. Allen\*

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[dx.doi.org/10.1021/jp5062094](https://doi.org/10.1021/jp5062094)**Origin of the High Activity of Mesoporous  $\text{CeO}_2$  Supported Monomeric  $\text{VO}_x$  for Low-Temperature Gas-Phase Selective Oxidative Dehydrogenation of Benzyl Alcohol: Role As an Electronic "Hole"**

Juanjuan Liu, Xin-Ping Wu, Shihui Zou, Yihu Dai, Liping Xiao, Xue-Qing Gong,\* and Jie Fan\*

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[dx.doi.org/10.1021/jp506331u](https://doi.org/10.1021/jp506331u)**Modeling of Growth Morphology of Core–Shell Nanoparticles**

Vyacheslav Gorshkov, Vasily Kuzmenko, and Vladimir Privman\*

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[dx.doi.org/10.1021/jp506867n](https://doi.org/10.1021/jp506867n)**Three-Dimensional Organization of Surface-Bound Silicone Nanofilaments Revealed by Focused Ion Beam Nanotomography**

Georg R. Meseck, Andres Käch, and Stefan Seeger\*

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[dx.doi.org/10.1021/jp5069895](https://doi.org/10.1021/jp5069895)**Stability and Electronic Properties of Biphenylene Based Functionalized Nanoribbons and Sheets**

Pablo A. Denis\*

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[dx.doi.org/10.1021/jp507051q](https://doi.org/10.1021/jp507051q)**Chalcogen Atom Interaction with Palladium and the Complex Molecule–Metal Interface in Thiol Self Assembly**

Juanjuan Jia, Azzedine Bendounan, Karine Chaouchi, Stefan Kubsky, Fausto Sirotti, Luca Pasquali, and Vladimir A. Esaulov\*

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[dx.doi.org/10.1021/jp507072p](https://doi.org/10.1021/jp507072p)**Scanning Tunneling Microscope and Photoemission Spectroscopy Investigations of Bismuth on Epitaxial Graphene on  $\text{SiC}(0001)$** 

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[dx.doi.org/10.1021/jp507164c](https://doi.org/10.1021/jp507164c)**Probing the Hydrophobic Interaction between Air Bubbles and Partially Hydrophobic Surfaces Using Atomic Force Microscopy**

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[dx.doi.org/10.1021/jp507189n](https://doi.org/10.1021/jp507189n)**Surfaces of Rutile MnO<sub>2</sub> Are Electronically Conducting, Whereas the Bulk Material Is Insulating**

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[dx.doi.org/10.1021/jp507443k](https://doi.org/10.1021/jp507443k)**CO<sub>2</sub> Capture by TiO<sub>2</sub> Anatase Surfaces: A Combined DFT and FTIR Study**

Lorenzo Mino, Giuseppe Spoto, and Anna Maria Ferrari\*

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[dx.doi.org/10.1021/jp507585a](https://doi.org/10.1021/jp507585a)**Ultrafast Population Dynamics of Surface-Active Dyes during Electrochemically Controlled Ion Transfer across a Liquid/Liquid Interface**

Astrid J. Olaya, Pierre-François Brevet, Evgeny A. Smirnov, and Hubert H. Girault\*

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[dx.doi.org/10.1021/jp507590a](https://doi.org/10.1021/jp507590a)**Role of Silver Nanoparticles in Enhanced Xenon Adsorption Using Silver-Loaded Zeolites**

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[dx.doi.org/10.1021/jp507549v](https://doi.org/10.1021/jp507549v)**Electrosynthesis of Poly(alanine)-Like Peptides in Concentrated Alanine Based Electrolytes, Characterization Coupled to DFT Study and Application to pH Proton Receptor**

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[dx.doi.org/10.1021/jp5078328](https://doi.org/10.1021/jp5078328)**Reducing Band Gap and Enhancing Carrier Mobility of Boron Nitride Nanoribbons by Conjugated  $\pi$  Edge States**

Yu Wang, Yafei Li,\* and Zhongfang Chen\*

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[dx.doi.org/10.1021/jp507966v](https://doi.org/10.1021/jp507966v)**The Unique Properties of the Oxide-Metal Interface: Reaction of Ethanol on an Inverse Model CeO<sub>x</sub>-Au(111) Catalyst**

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[dx.doi.org/10.1021/jp508009x](https://doi.org/10.1021/jp508009x)**Primostrato Solid-State NMR Enhanced by Dynamic Nuclear Polarization: Pentacoordinated Al<sup>3+</sup> Ions Are Only Located at the Surface of Hydrated  $\gamma$ -Alumina**

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[dx.doi.org/10.1021/jp508141q](https://doi.org/10.1021/jp508141q)**Modeling Catalytic Steps on Extra-Framework Metal Centers in Zeolites. A Case Study on Ethylene Dimerization**

Shrabani Dinda, Agalya Govindasamy, Alexander Genest, and Notker Rösch\*

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Takashi Nishimura, Akira Sasahara, Hideyuki Murata, Toyoko Arai, and Masahiko Tomitori\*

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**Interaction of H<sub>2</sub> (D<sub>2</sub>) with OH (OD) Groups in a ZSM-5 Zeolite: FTIR Study of the Isotopic Effects**

Nikola Drenchev and Konstantin Hadjivanov\*

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**High-Pressure Phase Transition of Coffinite, USiO<sub>4</sub>**

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**Electronic Structure of FeSe<sub>1-x</sub>Te<sub>x</sub> Studied by X-ray Spectroscopy and Density Functional Theory**

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[dx.doi.org/10.1021/jp507210t](https://doi.org/10.1021/jp507210t)**Tunable Plasmon Resonance of Gold Nanoparticles Functionalized by Electroactive Bisthienylbenzene Oligomers or Polythiophene**

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[dx.doi.org/10.1021/jp507383w](https://doi.org/10.1021/jp507383w)**Excitation-Dependent Ultrafast Carrier Dynamics of Colloidal TiO<sub>2</sub> Nanorods in Organic Solvent**

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[dx.doi.org/10.1021/jp507411w](https://doi.org/10.1021/jp507411w)**Super Energy Absorption System Based on Nanofluidic Glycerol Solution**

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[dx.doi.org/10.1021/jp507487c](https://doi.org/10.1021/jp507487c)**Structural and Photoelectrochemical Properties of DC Magnetron-Sputtered TiO<sub>2</sub> Layers on FTO**

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**Intraexciton Transitions Observed in High Stability Doped Single-Wall Carbon Nanotube Films and Solutions**

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**Morphology and Emission Tuning in Fluorescent Nanoparticles Based on Phenylenediacetonitrile**

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**Strong Thermal Transport Anisotropy and Strain Modulation in Single-Layer Phosphorene**

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**Silicane as an Inert Substrate of Silicene: A Promising Candidate for FET**

Run-wu Zhang, Chang-wen Zhang,\* Wei-xiao Ji, Shu-jun Hu, Shi-shen Yan,\* Sheng-shi Li, Ping Li, Pei-ji Wang, and Yu-shen Liu

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**Preferential Location of Coinage Metal Dopants (M = Ag or Cu) in [Au<sub>25-x</sub>M<sub>x</sub>(SC<sub>2</sub>H<sub>4</sub>Ph)<sub>18</sub>]<sup>-</sup> (x ~ 1) As Determined by Extended X-ray Absorption Fine Structure and Density Functional Theory Calculations**

Seiji Yamazoe, Wataru Kurashige, Katsuyuki Nobusada, Yuichi Negishi, and Tatsuya Tsukuda\*