

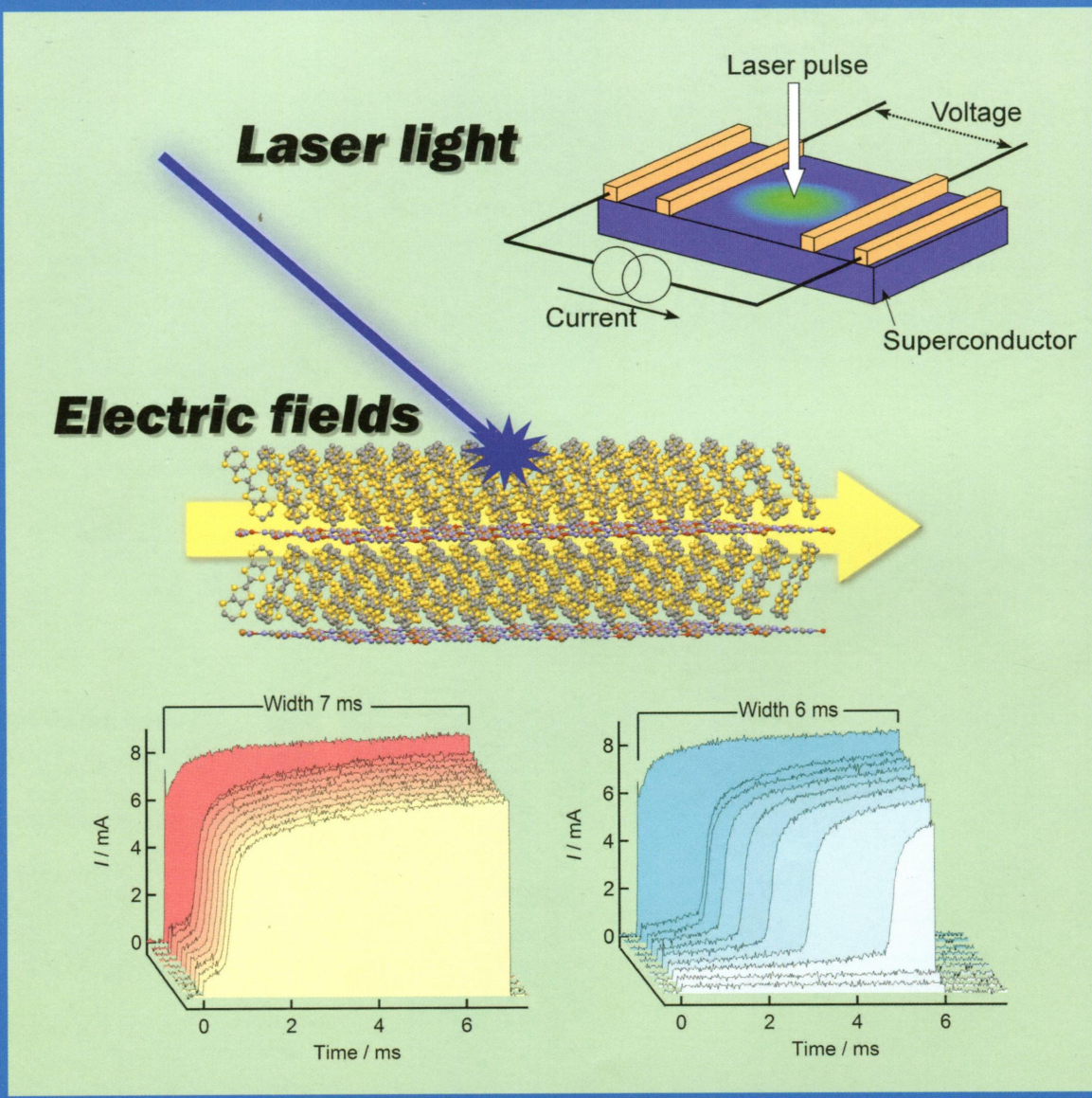
FLU  
J80/pc2

APRIL 10, 2014  
VOLUME 118  
NUMBER 14  
pubs.acs.org/JPCC

# THE JOURNAL OF PHYSICAL CHEMISTRY

# C

Tuning Function and  
Electron Dynamics in  
Molecular Conductors  
Using Photoirradiation  
and Electric Fields  
(see page 7251)



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



ACS Publications  
MOST TRUSTED. MOST CITED. MOST READ.

www.acs.org



**ON THE COVER:** Tuning function and electron dynamics in molecular conductors using photoirradiation and electric fields. Top right reproduced from: Iimori, T.; Sabeth, F.; Naito, T.; Ohta, N. Time-Resolved Photoresponse Measurements of the Electrical Conductivity of the Quasi-Two-Dimensional Organic Superconductor  $\beta$ -(BEDT-TTF) $_2$ I $_3$  Using a Nanosecond Laser Pulse. *J. Phys. Chem. C* **2011**, *115* (48), 23998–24003. Bottom graphs reproduced from: Iimori, T.; Naito, T.; Ohta, N. Unprecedented Optoelectronic Function in Organic Conductor: Memory Effect of Photoswitching Controlled by Voltage Pulse Width. *J. Phys. Chem. C* **2009**, *113* (11), 4654–4661. See page 7251.

## Feature Article

7251

[dx.doi.org/10.1021/jp4126123](http://dx.doi.org/10.1021/jp4126123)

**Tuning of Electrical Conductivity by Photoirradiation and Electric Fields**

Toshifumi Iimori and Nobuhiro Ohta\*

## Articles

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

7261



[dx.doi.org/10.1021/jp407736f](http://dx.doi.org/10.1021/jp407736f)

**Intrinsic Oxygen Vacancy and Extrinsic Aluminum Dopant Interplay: A Route to the Restoration of Defective TiO $_2$**

Conn O'Rourke\* and David R. Bowler

7272



[dx.doi.org/10.1021/jp409617r](http://dx.doi.org/10.1021/jp409617r)

**Determination of the Charge Transport Mechanisms in Ultrathin Copper Phthalocyanine Vertical Heterojunctions**

Carlos C. Bof Bufon,\* Céline Vervacke, Dominic J. Thurner, Michael Fronk, Georgeta Salvan, Susi Lindner, Martin Knupfer, Dietrich R. T. Zahn, and Oliver G. Schmidt

7280



[dx.doi.org/10.1021/jp410193m](http://dx.doi.org/10.1021/jp410193m)

**High Pressure Equilibria of Dimethylamine Borane, Dihydridobis(dimethylamine)boron(III) Tetrahydridoborate(III), and Hydrogen**

Robert G. Potter,\* Maddury Somayazulu,\* George Cody, and Russell J. Hemley






7288



[dx.doi.org/10.1021/jp4120157](http://dx.doi.org/10.1021/jp4120157)

**Coupling of Organic and Inorganic Vibrational States and Their Thermal Transport in Nanocrystal Arrays**

Wee-Liat Ong, Shubhaditya Majumdar, Jonathan A. Malen, and Alan J. H. McGaughey\*

- 7296  [dx.doi.org/10.1021/jp412038y](https://doi.org/10.1021/jp412038y)  
**Poly(3,4-ethylenedioxythiophene) Sheath Over a SnO<sub>2</sub> Hollow Spheres/Graphene Oxide Hybrid for a Durable Anode in Li-Ion Batteries**  
Akkisetty Bhaskar, Melepurath Deepa,\* M. Ramakrishna, and T. N. Rao
- 7307  [dx.doi.org/10.1021/jp412087f](https://doi.org/10.1021/jp412087f)  
**Physicochemical Investigation of the Panchromatic Effect on  $\beta$ -Substituted Zn<sup>II</sup> Porphyrinates for DSSCs: The Role of the  $\pi$  Bridge between a Dithienylethylene Unit and the Porphyrinic Ring**  
Gabriele Di Carlo, Alessio Orbelli Biroli, Francesca Tessore, Maddalena Pizzotti,\* Patrizia Romana Mussini, Anna Amat, Filippo De Angelis, Alessandro Abboto, Vanira Trifiletti, and Riccardo Ruffo
- 7321 [dx.doi.org/10.1021/jp412354f](https://doi.org/10.1021/jp412354f)  
**Versatile Energetic Behavior of ZIF-8 upon High Pressure Intrusion–Extrusion of Aqueous Electrolyte Solutions**  
Guillaume Ortiz, Habiba Nouali, Claire Marichal, Gérald Chaplais,\* and Joël Patarin\*
- 7329  [dx.doi.org/10.1021/jp4123979](https://doi.org/10.1021/jp4123979)  
**Hydrophobic Carbon-Doped TiO<sub>2</sub>/MCF-F Composite as a High Performance Photocatalyst**  
Dianyu Qi, Mingyang Xing, and Jinlong Zhang\*
- 7337  [dx.doi.org/10.1021/jp500132w](https://doi.org/10.1021/jp500132w)  
**Mechanisms of Photogeneration and Relaxation of Excitons and Mobile Carriers in Anatase TiO<sub>2</sub>**  
Maria C. Fravventura, Laurens D. A. Siebbeles, and Tom J. Savenije\*
- 7344  [dx.doi.org/10.1021/jp500597m](https://doi.org/10.1021/jp500597m)  
**Influence of Gold Nanoparticles Anchored to Carbon Nanotubes on Formation and Decomposition of Li<sub>2</sub>O<sub>2</sub> in Nonaqueous Li–O<sub>2</sub> Batteries**  
Wugang Fan, Xiangxin Guo,\* Dongdong Xiao, and Lin Gu
- 7351 [dx.doi.org/10.1021/jp500905u](https://doi.org/10.1021/jp500905u)  
**Insights into Changes of Lattice and Electronic Structure Associated with Electrochemistry of Li<sub>2</sub>CoSiO<sub>4</sub> Polymorphs**  
Caixia Zhang, Zhenlian Chen, Yongzhi Zeng, Zhifeng Zhang, and Jun Li\*
- 7357 [dx.doi.org/10.1021/jp5011023](https://doi.org/10.1021/jp5011023)  
**Straightforward Approach toward SiO<sub>2</sub> Nanospheres and Their Superior Lithium Storage Performance**  
Jiguo Tu, Yan Yuan, Pan Zhan, Handong Jiao, Xindong Wang, Hongmin Zhu, and Shuqiang Jiao\*
- 7363 [dx.doi.org/10.1021/jp501970j](https://doi.org/10.1021/jp501970j)  
**Generation of Cathode Passivation Films via Oxidation of Lithium Bis(oxalato) Borate on High Voltage Spinel (LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub>)**  
Mengqing Xu, Nikolaos Tsiouvaras, Arnd Garsuch, Hubert A. Gasteiger, and Brett L. Lucht\*

## Surfaces, Interfaces, Porous Materials, and Catalysis

- 7369  [dx.doi.org/10.1021/jp4096776](https://doi.org/10.1021/jp4096776)  
**Fluorine-Modified Porous Graphene as Membrane for CO<sub>2</sub>/N<sub>2</sub> Separation: Molecular Dynamic and First-Principles Simulations**  
Tiantian Wu, Qingzhong Xue,\* Cuicui Ling, Meixia Shan, Zilong Liu, Yehan Tao, and Xiaofang Li
- 7377  [dx.doi.org/10.1021/jp410293j](https://doi.org/10.1021/jp410293j)  
**Synthesis of Vertically Conformal ZnO/CuO Core–Shell Nanowire Arrays by Electrophoresis-Assisted Electroless Deposition**  
Sanggon Kim, Younghyo Lee, Ayeong Gu, Chanseok You, Kwangjoong Oh, Sanghyun Lee, and Yeonho Im\*
- 7386 [dx.doi.org/10.1021/jp410848f](https://doi.org/10.1021/jp410848f)  
**Insights into the WO<sub>x</sub> Coverage-Dependent Location and Oxidation State of Noble Metals Supported on Tungstated Oxides: The Case of Rh/WO<sub>x</sub>–Ce<sub>0.62</sub>Zr<sub>0.38</sub>O<sub>2</sub>**  
Thomas Bonnotte, Rachel P. Doherty, Céline Sayag, Jean-Marc Krafft, Christophe Méthivier, Mickaël Sicard, Frédéric Ser, and Cyril Thomas\*
- 7398  [dx.doi.org/10.1021/jp411523g](https://doi.org/10.1021/jp411523g)  
**Adsorption of Glyoxal (CHOCHO) and Its UV Photolysis Products on the Surface of Atmospheric Ice Nanoparticles. DFT and Density Functional Tight-Binding Study**  
Stanislav K. Ignatov,\* Oleg B. Gadzhiev, Alexey G. Razuvaev, Artëm E. Masunov, and Otto Schrems
- 7414 [dx.doi.org/10.1021/jp411730z](https://doi.org/10.1021/jp411730z)  
**The Role of Adsorbed Ions during Electrocatalysis in Ionic Liquids**  
Andinet Ejigu and Darren A. Walsh\*
- 7423  [dx.doi.org/10.1021/jp500037z](https://doi.org/10.1021/jp500037z)  
**Adsorption and Dynamics in Hierarchical Metal–Organic Frameworks**  
François Villemot, Anne Galameau, and Benoit Coasne\*
- 7434  [dx.doi.org/10.1021/jp500116n](https://doi.org/10.1021/jp500116n)  
**Photocatalytic Removal of NO<sub>x</sub> over Visible Light Responsive Oxygen-Deficient TiO<sub>2</sub>**  
Jin Zhu Ma, Hongmin Wu, Yongchun Liu, and Hong He\*
- 7442  [dx.doi.org/10.1021/jp500178y](https://doi.org/10.1021/jp500178y)  
**Improved Interaction of Hydrogen on Transition-Metal-Doped Al(100) Stepped Surface**  
M. M. Zheng, T. Q. Ren, G. Chen,\* and Y. Kawazoe
- 7451 [dx.doi.org/10.1021/jp5004775](https://doi.org/10.1021/jp5004775)  
**Band Structure Tuning of TiO<sub>2</sub> for Enhanced Photoelectrochemical Water Splitting**  
Jiajun Wang, Haifeng Sun, Jing Huang, Qunxiang Li,\* and Jinlong Yang

7458  [dx.doi.org/10.1021/jp5005133](https://doi.org/10.1021/jp5005133)

**Flexible Structure of a Thermally Stable Hybrid Aluminosilicate Built with Only the Three-Ring Unit**

Michela Bellettato,\* Lucia Bonoldi, Giuseppe Cruciani, Cristina Flego, Stefania Guidetti, Roberto Millini, Erica Montanari, Wallace O'Neil Parker Jr., and Stefano Zanardi\*

7468  [dx.doi.org/10.1021/jp500537v](https://doi.org/10.1021/jp500537v)

**Mechanistic Evidence for Sequential Displacement–Reduction Routes in the Synthesis of Pd–Au Clusters with Uniform Size and Clean Surfaces**

Sebastian Kunz and Enrique Iglesia\*

7480 [dx.doi.org/10.1021/jp500579b](https://doi.org/10.1021/jp500579b)

**Control of Gas Flow in Narrow Channels Using an Electric Field To Modify the Flow Boundary Condition**

Dongjin Seo and William A. Ducker\*

7489 [dx.doi.org/10.1021/jp5012318](https://doi.org/10.1021/jp5012318)

**Electron Transport Properties of Au, Ag, and Cu Atomic Contacts in a Hydrogen Environment**

Tomoka Nakazumi, Satoshi Kaneko, and Manabu Kiguchi\*

7494 [dx.doi.org/10.1021/jp501268y](https://doi.org/10.1021/jp501268y)

**Switchable Silver Nanostructures Controlled with an Atomic Force Microscope**

S. Bakhti, S. Biswas, C. Hubert, S. Reynaud, F. Vocanson, and N. Destouches\*

7501  [dx.doi.org/10.1021/jp501611t](https://doi.org/10.1021/jp501611t)

**Effect of Silicon Doping on the Reactivity and Catalytic Activity of Gold Clusters**

Dar Manzoor, Sailaja Krishnamurty, and Sourav Pal\*

7508  [dx.doi.org/10.1021/jp502387x](https://doi.org/10.1021/jp502387x)

**Ring Current Effects: Factors Affecting the NMR Chemical Shift of Molecules Adsorbed on Porous Carbons**

Alexander C. Forse, John M. Griffin, Volker Presser, Yuri Gogotsi, and Clare P. Grey\*

**Plasmonics, Optical Materials, and Hard Matter**

7515 [dx.doi.org/10.1021/jp4081965](https://doi.org/10.1021/jp4081965)










**Red Photoluminescence from Bi<sup>3+</sup> and the Influence of the Oxygen-Vacancy Perturbation in ScVO<sub>4</sub>: A Combined Experimental and Theoretical Study**

Fengwen Kang, Xiaobao Yang, Mingying Peng,\* Lothar Wondraczek, Zhijun Ma, Qinyuan Zhang, and Jianrong Qiu

7523  [dx.doi.org/10.1021/jp4112124](https://doi.org/10.1021/jp4112124)

**Gold Nanoparticle–Polydimethylsiloxane Thin Films Enhance Thermoplasmonic Dissipation by Internal Reflection**

Jeremy R. Dunklin, Gregory T. Forcherio, Keith R. Berry Jr., and D. K. Roper\*

- 7532  [dx.doi.org/10.1021/jp411483x](https://doi.org/10.1021/jp411483x)  
**Assessment of Exchange-Correlation Functionals in Reproducing the Structure and Optical Gap of Organic-Protected Gold Nanoclusters**  
Francesco Muniz-Miranda,\* Maria Cristina Menziani, and Alfonso Pedone
- 7545  [dx.doi.org/10.1021/jp412204f](https://doi.org/10.1021/jp412204f)  
**Zinc Induced a Dramatic Enhancement of the Nonlinear Optical Properties of an Azo-Based Iminopyridine Ligand**  
Imen Guezguez, Awatef Ayadi, Karolina Ordon, Konstantinos Iliopoulos, Diana G. Branzea, Anna Migalska-Zalas, Malgorzata Makowska-Janusik, Abdelkrim El-Ghayoury,\* and Bouchta Sahraoui\*
- 7554  [dx.doi.org/10.1021/jp412329x](https://doi.org/10.1021/jp412329x)  
**Electrostatic Control of Orbital Ordering in Noncubic Crystals**  
Pablo García-Fernández,\* Miguel Moreno, and José A. Aramburu
- 7562  [dx.doi.org/10.1021/jp412366y](https://doi.org/10.1021/jp412366y)  
**Pure Hexagonal Phase of  $\text{EuF}_3$  Modulated by High Pressure**  
Qian Li, Shourui Li, Kai Wang,\* Jing Liu, Bingbing Liu, Ke Yang, and Bo Zou\*
- 7569  [dx.doi.org/10.1021/jp412614k](https://doi.org/10.1021/jp412614k)  
**Molecular Understanding of the Chemical Stability of Organic Materials for OLEDs: A Comparative Study on Sulfonyl, Phosphine-Oxide, and Carbonyl-Containing Host Materials**  
Na Lin, Juan Qiao,\* Lian Duan, Liduo Wang, and Yong Qiu
- 7579  [dx.doi.org/10.1021/jp4126792](https://doi.org/10.1021/jp4126792)  
**Two-Dimensional Plasmonic Superlattice Based on Au Nanoparticles Self-Assembling onto a Functionalized Substrate**  
Michela Corricelli, Nicoletta Depalo, Elisabetta Fanizza, Davide Altamura, Cinzia Giannini, Dritan Siliqi, Rosa Di Mundo, Fabio Palumbo, Vasily G. Kravets, Alexander N. Grigorenko, Angela Agostiano, Marinella Striccoli, and M. Lucia Curri\*
- 7591  [dx.doi.org/10.1021/jp412702g](https://doi.org/10.1021/jp412702g)  
**Tunable Luminescence and  $\text{Ce}^{3+} \rightarrow \text{Tb}^{3+} \rightarrow \text{Eu}^{3+}$  Energy Transfer of Broadband-Excited and Narrow Line Red Emitting  $\text{Y}_2\text{SiO}_5:\text{Ce}^{3+}, \text{Tb}^{3+}, \text{Eu}^{3+}$  Phosphor**  
Xinguo Zhang,\* Liya Zhou, Qi Pang, Jianxin Shi, and Menglian Gong
- 7599  [dx.doi.org/10.1021/jp412798u](https://doi.org/10.1021/jp412798u)  
**Plasmon Controlled Exciton Fluorescence of Molecular Aggregates**  
Alexander V. Sorokin,\* Alexander A. Zabolotskii, Nikita V. Pereverzev, Svetlana L. Yefimova, Yury V. Malyukin, and Alexander I. Plekhanov
- 7606  [dx.doi.org/10.1021/jp500009k](https://doi.org/10.1021/jp500009k)  
**Optical Generation of Hot Plasmonic Carriers in Metal Nanocrystals: The Effects of Shape and Field Enhancement**  
Hui Zhang and Alexander O. Govorov\*

7615 

[dx.doi.org/10.1021/jp501237c](https://doi.org/10.1021/jp501237c)

**DFT-D3 Study of Some Molecular Crystals**  
Jonas Moellmann and Stefan Grimme\*

## Physical Processes in Nanomaterials and Nanostructures

7622

[dx.doi.org/10.1021/jp410805q](https://doi.org/10.1021/jp410805q)

**Melting Behavior of Aluminum Nanowires in Carbon Nanotubes**  
R. R. Fang, Y. Z. He, K. Zhang, and H. Li\*

7630

[dx.doi.org/10.1021/jp411250c](https://doi.org/10.1021/jp411250c)

**Effects of Crystallographic and Shape Anisotropies on Dopant-Carrier Exchange Interactions in Magnetic Semiconductor Quantum Dots**  
Bo Peng, Joseph W. May, Daniel R. Gamelin,\* and Xiaosong Li\*

7637 

[dx.doi.org/10.1021/jp411348f](https://doi.org/10.1021/jp411348f)

**Electron Transfer from Graphene Quantum Dots to the Copper Complex Enhances Its Nuclease Activity**  
Bin Zheng, Chong Wang, Xiaozhen Xin, Fei Liu, Xuejiao Zhou, Jingyan Zhang,\* and Shouwu Guo\*

7643 

[dx.doi.org/10.1021/jp411572x](https://doi.org/10.1021/jp411572x)

**Coherent Electron Transmission across Nanographenes Tethered to Gold Electrodes: Influence of Linker Topology, Ribbon Width, and Length**  
Silvio Osella, Victor Geskin, Jérôme Cornil, and David Beljonne\*

7653 

[dx.doi.org/10.1021/jp412145j](https://doi.org/10.1021/jp412145j)

**Role of Nanoparticle Selectivity in the Symmetry Breaking of Cylindrically Confined Block Copolymers**  
Jay Hoon Park, Jun Yin, Vibha Kalra, and Yong Lak Joo\*

7669 

[dx.doi.org/10.1021/jp500013g](https://doi.org/10.1021/jp500013g)

**Do Excited Silicon–Oxygen Double Bonds Emit Light?**  
Yinan Shu and Benjamin G. Levine\*

7678 

[dx.doi.org/10.1021/jp500227s](https://doi.org/10.1021/jp500227s)

**Single Crystallization of Olivine Lithium Phosphate Nanowires using Oriented Attachments**  
Jun Kikkawa,\* Eiji Hosono,\* Masashi Okubo, Koichi Kagesawa, Haoshen Zhou, Takuro Nagai, and Koji Kimoto

7683

[dx.doi.org/10.1021/jp500431k](https://doi.org/10.1021/jp500431k)

**High Pressure Raman and X-ray Diffraction Study of [121] Tetramantane**  
Fan Yang, Yu Lin, Jeremy E. P. Dahl, Robert M. K. Carlson, and Wendy L. Mao\*

7690

[dx.doi.org/10.1021/jp500570f](https://doi.org/10.1021/jp500570f)**Polyethylene-glycol-Stabilized Ag Nanoparticles for Surface-Enhanced Raman Scattering Spectroscopy: Ag Surface Accessibility Studied Using Metalation of Free-Base Porphyrins**

Petra Šimáková, Juliette Gautier, Marek Procházka,\* Katel Hervé-Aubert, and Igor Chourpa

7698

[dx.doi.org/10.1021/jp500580g](https://doi.org/10.1021/jp500580g)**Statistical Raman Microscopy and Atomic Force Microscopy on Heterogeneous Graphene Obtained after Reduction of Graphene Oxide**

Siegfried Eigler,\* Ferdinand Hof, Michael Enzelberger-Heim, Stefan Grimm, Paul Müller, and Andreas Hirsch

7705

[dx.doi.org/10.1021/jp500701b](https://doi.org/10.1021/jp500701b)**Competing Occupation of Guest Molecules in Hydroquinone Clathrates Formed from Binary C<sub>2</sub>H<sub>4</sub> and CH<sub>4</sub> Gas Mixtures**

Jong-Won Lee, Seong-Pil Kang,\* and Ji-Ho Yoon\*

7710

[dx.doi.org/10.1021/jp500761f](https://doi.org/10.1021/jp500761f)**Electron-Transfer Reduction Properties and Excited-State Dynamics of Benzo[ghi]peryleneimide and Coroneneimide Derivatives**

Koichi Ida, Hayato Sakai, Kei Ohkubo, Yasuyuki Araki,\* Takehiko Wada, Tomo Sakanoue, Taishi Takenobu,\* Shunichi Fukuzumi,\* and Taku Hasobe\*

7721

[dx.doi.org/10.1021/jp5014253](https://doi.org/10.1021/jp5014253)**Particle Size Effects on Charge Ordering and Exchange Bias in Nanosized Sm<sub>0.43</sub>Ca<sub>0.57</sub>MnO<sub>3</sub>**

Vladimir Markovich,\* Roman Puzniak, Ivan Fita, Dmitrii Mogilyansky, Andrzej Wisniewski, Gad Gorodetsky, and Grzegorz Jung

7730

[dx.doi.org/10.1021/jp502102a](https://doi.org/10.1021/jp502102a)**Connecting the Dots: The Kinetics and Thermodynamics of Hot, Cold, and Surface-Trapped Excitons in Semiconductor Nanocrystals**

Jonathan Mooney, Michael M. Krause, and Patanjali Kambhampati\*