

APRIL 4, 2013

VOLUME 117

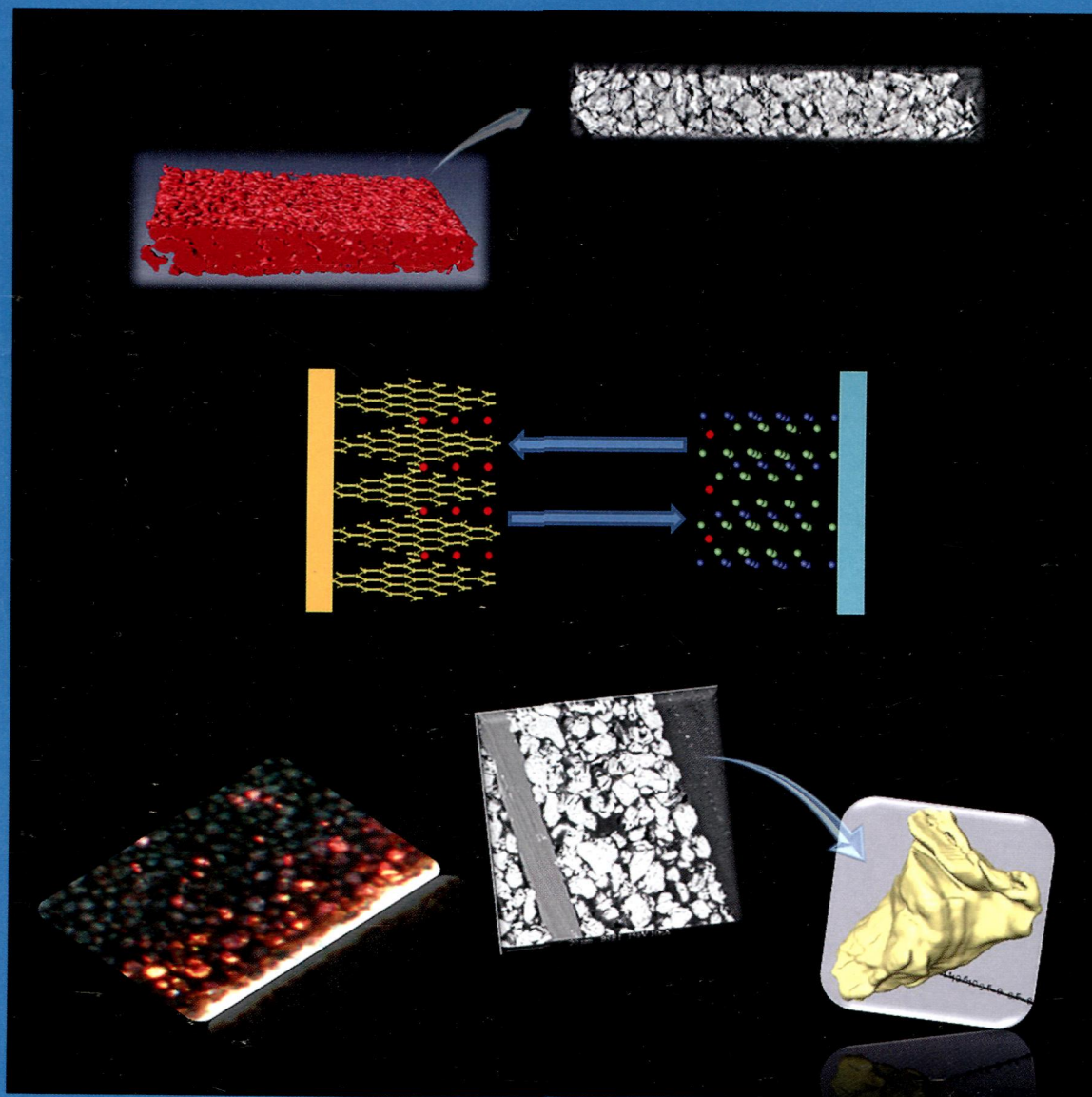
NUMBER 13

pubs.acs.org/JPCC

# THE JOURNAL OF PHYSICAL CHEMISTRY

# C

Mesoscale Complexity  
and Inhomogeneity in  
Li-ion Batteries  
(see page 5A)



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:** Mesoscale complexity and inhomogeneity in Li-ion batteries. Most Li-ion battery failures can be ascribed to the presence of nano- and microscale inhomogeneities that interact at the mesoscale. In an ideal Li-ion battery, the only steps that should occur are Li moving back and forth between and into the electrodes. In contrast, in a failed battery, inhomogeneities (regions with sharply varying mechanical, electrical, morphological, or chemical properties, including interfaces) act by hindering Li transport so that Li does not get to the right place at the right time. A detailed understanding of the electrode structures and inhomogeneities at all scales, from nano- to mesoscale (where inhomogeneities interact), can lead to improved understanding of durability and failure mechanisms, ultimately leading to longer-lived batteries, with all of their attendant advantages. See page 6481.

## Feature Article

6481 [dx.doi.org/10.1021/jp3111431z](https://doi.org/10.1021/jp3111431z)  
**Effects of Inhomogeneities—Nanoscale to Mesoscale—on the Durability of Li-Ion Batteries**  
Stephen J. Harris and Peng Lu\*

## Articles

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

6493 [dx.doi.org/10.1021/jp308976u](https://doi.org/10.1021/jp308976u)  
**High CO<sub>2</sub> Selectivity of ZnO Powder Catalysts for Methanol Steam Reforming**  
Barr Halevi, Sen Lin, Aaron Roy, He Zhang, Ese Jeroro, John Vohs, Yong Wang, Hua Guo, and Abhaya K. Datye\*

6504 [dx.doi.org/10.1021/jp312410t](https://doi.org/10.1021/jp312410t)  
**Understanding the Conduction Mechanism of the Protonic Conductor C<sub>5</sub>H<sub>2</sub>PO<sub>4</sub> by Solid-State NMR Spectroscopy**  
Gunwoo Kim, Frédéric Blanc, Yan-Yan Hu, and Clare P. Grey\*

6516 [dx.doi.org/10.1021/jp312613r](https://doi.org/10.1021/jp312613r)  
**Tuning the Electronic Structure of Graphite Oxide through Ammonia Treatment for Photocatalytic Generation of H<sub>2</sub> and O<sub>2</sub> from Water Splitting**  
Te-Fu Yeh, Shean-Jen Chen, Chen-Sheng Yeh, and Hsisheng Teng\*

6525 [dx.doi.org/10.1021/jp312658q](https://doi.org/10.1021/jp312658q)  
**Examining Hysteresis in Composite xLi<sub>2</sub>MnO<sub>3</sub>·(1-x)LiMO<sub>2</sub> Cathode Structures**  
Jason R. Croy,\* Kevin G. Gallagher, Mahalingam Balasubramanian, Zonghai Chen, Yang Ren, Donghan Kim, Sun-Ho Kang, Dennis W. Dees, and Michael M. Thackeray

6537 dx.doi.org/10.1021/jp4001237  
**Solution-Processed High-Detectivity Near-Infrared Polymer Photodetectors Fabricated by a Novel Low-Bandgap Semiconducting Polymer**  
Xiaowen Hu, Yang Dong, Fei Huang,\* Xiong Gong,\* and Yong Cao

6544 dx.doi.org/10.1021/jp400782g  
**Concentration and Solvent Effects on the Excited State Dynamics of the Solar Cell Dye D149: The Special Role of Protons**  
Ahmed M. El-Zohry and Burkhard Zietz\*

6554 dx.doi.org/10.1021/jp400961k  
**Rubidium Hydride: An Exceptional Dehydrogenation Catalyst for the Lithium Amide/Magnesium Hydride System**  
Tolulope Durojaiye, Jalaal Hayes, and Andrew Goudy\*

6561 dx.doi.org/10.1021/jp401032c  
**NiS<sub>2</sub>/Reduced Graphene Oxide Nanocomposites for Efficient Dye-Sensitized Solar Cells**  
Zhuoqun Li, Feng Gong, Gang Zhou, and Zhong-Sheng Wang\*

## Surfaces, Interfaces, Porous Materials, and Catalysis

6567 dx.doi.org/10.1021/jp311015w  
**Fluorescence Quenching of 5,5'-Disulfopropyl-3,3'-dichlorothiocyanine Dye Adsorbed on Gold Nanoparticles**  
Ana Vujačić, Vesna Vasić, Miroslav Dramićanin, Soñja P. Sovilj, Nataša Bibić, Slobodan Milonjić, and Vesna Vodnik\*

6578 dx.doi.org/10.1021/jp311285g  
**Solid State Structural Transformation of Tetraborate into Monoborate in the Interlayer Galleries of Reconstructed ZnAl Layered Double Hydroxide**  
Paulmanickam Koilraj, Rajendra Singh Thakur, and Kannan Srinivasan\*

6587 dx.doi.org/10.1021/jp311481d  
**Dimethyl Disulfide on Cu(111): From Nondissociative to Dissociative Adsorption**  
Xiao-Li Fan,\* Yan Liu, Run-Xin Ran, and Woon-Ming Lau\*

6594 dx.doi.org/10.1021/jp311701r  
**Insight into the Preference Mechanism of CH<sub>x</sub> (x = 1–3) and C–C Chain Formation Involved in C<sub>2</sub> Oxygenate Formation from Syngas on the Cu(110) Surface**  
Riguang Zhang, Xuancheng Sun, and Baojun Wang\*

6607 dx.doi.org/10.1021/jp3123117  
**Capacitive Composites Made of Conducting Polymer and Lysozyme: Toward the Biocondenser**  
Daniel E. López-Pérez, David Aradilla, Luis J. del Valle, and Carlos Alemán\*

6620 dx.doi.org/10.1021/jp312501b  
**Adsorption of Water–Acetonitrile Mixtures to Model Silica Surfaces**  
Sergey M. Melnikov, Alexandra Hóltzel, Andreas Seidel-Morgenstern, and Ulrich Tallarek\*

6632 dx.doi.org/10.1021/jp312569q  
**Azimuthal Dichroism in Near-Edge X-ray Absorption Fine Structure Spectra of Planar Molecules**  
Guido Fratesi,\* Valeria Lanzilotto, Luca Floreano, and Gian Paolo Brivio

6639 dx.doi.org/10.1021/jp312645f  
**Ab Initio Prediction of Surface Stability of Fluorite Materials and Experimental Verification**  
P. Maldonado,\* J. R. A. Godinho, L. Z. Evins, and P. M. Oppeneer

6651 dx.doi.org/10.1021/jp312649a  
**Single Collision Events of Conductive Nanoparticles Driven by Migration**  
Jun Hui Park, Aliaksei Boika, Hyun S. Park, Heung Chan Lee, and Allen J. Bard\*

6658 dx.doi.org/10.1021/jp312650f  
**Shape of Water–Air Interface beneath a Drop on a Superhydrophobic Surface Revealed: Constant Curvature That Approaches Zero**  
Boris Haimov, Sasha Pechook, Orna Ternyak, and Boaz Pokroy\*

6664 dx.doi.org/10.1021/jp312733t  
**Structural Characterization of Unprecedented Al<sub>14</sub>O<sup>−</sup> and Al<sub>15</sub>O<sub>2</sub><sup>−</sup>: Photoelectron Spectroscopy and Density Functional Calculations**  
Tomomi Watanabe and Tatsuya Tsukuda\*

6669 dx.doi.org/10.1021/jp400193k  
**Redox State Sensitive Spectroscopy of the Model Compound [(H-dcbpy)<sub>2</sub>Ru<sup>II</sup>(NCS)<sub>2</sub>]<sup>2−</sup> (dcbpy = 2,2'-Bipyridine-4,4'-dicarboxylate)**  
Linda Zedler, Julien Guthmuller, Inês Rabelo de Moraes, Sven Kriek, Michael Schmitt, Jürgen Popp, and Benjamin Dietzek\*

6678 dx.doi.org/10.1021/jp4003627  
**Surface Transformations and Water Uptake on Liquid and Solid Butanol near the Melting Temperature**  
Panos Papagiannakopoulos,\* Xiangrui Kong, Erik S. Thomson, Nikola Marković, and Jan B. C. Pettersson\*

6686 dx.doi.org/10.1021/jp400565m  
**Strategies for the Immobilization of Bacteriophages on Gold Surfaces Monitored by Surface Plasmon Resonance and Surface Morphology**  
Nancy Tawil, Edward Sacher,\* Rosemonde Mandeville, and Michel Meunier

6692 [dx.doi.org/10.1021/jp400798q](https://doi.org/10.1021/jp400798q)  
**Reaction of CO, CH<sub>2</sub>O, CH<sub>3</sub>OH on Zn-Modified Pt(111) Surfaces**  
Eddie Martono and John M. Vohs\*

6702 [dx.doi.org/10.1021/jp400828v](https://doi.org/10.1021/jp400828v)  
**3D Organized Macroporous Bioactive Glasses: a Study of Pore Size Effect on Physicochemical Reactivity by Micro-PIXE-RBS**  
Jeremy Soulié,\* Adeline Hardy-Dessources, Jean-Marie Nedelec, and Edouard Jallot

6712 [dx.doi.org/10.1021/jp400873t](https://doi.org/10.1021/jp400873t)  
**Surface Plasmon Resonance Determination of the Binding Mechanisms of L-Cysteine and Mercaptoundecanoic Acid on Gold**  
Nancy Tawil, Ali Hatf, Edward Sacher,\* Mathieu Maisonneuve, Thomas Gervais, Rosemonde Mandeville, and Michel Meunier

6719 [dx.doi.org/10.1021/jp401532x](https://doi.org/10.1021/jp401532x)  
**Adsorption of Aromatic Hydrocarbon Molecules at the Surface of Ice, As Seen by Grand Canonical Monte Carlo Simulation**  
Zsuzsanna E. Mészár, György Hantal, Sylvain Picaud,\* and Pál Jedlovsky\*

## Plasmonics, Optical Materials, and Hard Matter

6730 [dx.doi.org/10.1021/jp310475d](https://doi.org/10.1021/jp310475d)  
**Hole Transport in Diketopyrrolopyrrole (DPP) Small Molecules: A Joint Theoretical and Experimental Study**  
Zi Li, Xu Zhang, Yuan Zhang, Cristiano F. Woellner, Martijn Kuik, Jianhua Liu, Thuc-Quyen Nguyen, and Gang Lu\*

6741 [dx.doi.org/10.1021/jp310514z](https://doi.org/10.1021/jp310514z)  
**Quantum Size Effects in the Optical Properties of Ligand Stabilized Aluminum Nanoclusters**  
Sukhendu Mandal, Juan Wang, Randall E. Winans, Lasse Jensen,\* and Ayusman Sen\*

6747 [dx.doi.org/10.1021/jp400476m](https://doi.org/10.1021/jp400476m)  
**Sharp Fickian Behavior of Electrogenenerated Chemiluminescence Waves in Conjugated Polymer Films**  
David A. Edwards\*

6752 [dx.doi.org/10.1021/jp400788h](https://doi.org/10.1021/jp400788h)  
**pH and Temperature Modulated Aggregation of Hydrophilic Gold Nanorods with Perylene Dyes and Carbon Nanotubes**  
Chenming Xue, Ozgul Birel, Yuhua Xue, Liming Dai, Augustine Urbas, and Quan Li\*

6759 [dx.doi.org/10.1021/jp4011839](https://doi.org/10.1021/jp4011839)  
**Energy-Transfer-Upconversion Models, Their Applicability and Breakdown in the Presence of Spectroscopically Distinct Ion Classes: A Case Study in Amorphous Al<sub>2</sub>O<sub>3</sub>:Er<sup>3+</sup>**  
L. Agazzi, K. Wörhoff, and M. Pollnau\*

## Physical Processes in Nanomaterials and Nanostructures

6777 [dx.doi.org/10.1021/jp311641g](https://doi.org/10.1021/jp311641g)  
**Thermodynamic Control of Metal Loading and Composition of Carbon Aerogel Supported Pt–Cu Alloy Nanoparticles by Supercritical Deposition**  
S. E. Bozbag, U. Unal, M. A. Kurykin, C. J. Ayala, M. Aindow, and C. Erkey\*

6788 [dx.doi.org/10.1021/jp311727t](https://doi.org/10.1021/jp311727t)  
**Tuning Radical Species in Graphene Oxide in Aqueous Solution by Photoirradiation**  
Xue-Liang Hou, Jing-Liang Li, Simon C. Drew, Bin Tang, Lu Sun,\* and Xun-Gai Wang\*

6794 [dx.doi.org/10.1021/jp312321t](https://doi.org/10.1021/jp312321t)  
**Effect of Electrolyte Conductivity on Controlled Electrochemical Synthesis of Zinc Oxide Nanotubes and Nanorods**  
Marwa Abd-Allah, Nafiseh Moghimi, Lei Zhang, Nina F. Heinig, Liyan Zhao, Joseph P. Thomas, and K. T. Leung\*

6800 [dx.doi.org/10.1021/jp312438u](https://doi.org/10.1021/jp312438u)  
**Effect of Rotational Degrees of Freedom on Molecular Mobility**  
M. Jafary-Zadeh, C. D. Reddy, and Yong-Wei Zhang\*


6807 [dx.doi.org/10.1021/jp312788k](https://doi.org/10.1021/jp312788k)  
**Phosphorus and Boron Codoped Colloidal Silicon Nanocrystals with Inorganic Atomic Ligands**  
Hiroshi Sugimoto, Minoru Fujii,\* Kenji Imakita, Shinji Hayashi, and Kensuke Akamatsu


6814 [dx.doi.org/10.1021/jp400208a](https://doi.org/10.1021/jp400208a)  
**Structure and Band Edge Energy of Highly Luminescent CdSe<sub>1-x</sub>Te<sub>x</sub> Alloyed Quantum Dots**  
Bo Hou, David Parker, Gabriela P. Kissling, Jonathan A. Jones, David Cherns, and David J. Fermin\*

6821 [dx.doi.org/10.1021/jp400223f](https://doi.org/10.1021/jp400223f)  
**Surface-Enhanced Raman Scattering in Purely Dielectric Structures via Bloch Surface Waves**  
S. Pirodda,\* X. G. Xu, A. Delfan, S. Mysore, S. Maiti, G. Dacarro, M. Patrini, M. Galli, G. Guizzetti, D. Bajoni, J. E. Sipe, G. C. Walker, and M. Liscidini


6826 [dx.doi.org/10.1021/jp4002753](https://doi.org/10.1021/jp4002753)  
**Stranski–Krastranov Shell Growth in ZnTe/CdSe Core/Shell Nanocrystals**  
Zhong-Jie Jiang and David F. Kelley\*


6835 [dx.doi.org/10.1021/jp4003388](https://doi.org/10.1021/jp4003388)  
**Spectroscopic Study of Electron and Hole Polarons in a High-Mobility Donor–Acceptor Conjugated Copolymer**  
Haihua Xu, Yuqian Jiang, Jun Li, Beng S. Ong, Zhigang Shuai, Jianbin Xu, and Ni Zhao\*


**6842**  dx.doi.org/10.1021/jp400559q  
**Nonlinear Optical Properties and Broadband Optical Power Limiting Action of Graphene Oxide Colloids**  
N. Liaros, P. Aloukos, A. Kolokithas-Ntoukas, A. Bakandritsos, T. Szabo, R. Zboril, and S. Couris\*

**6851**  dx.doi.org/10.1021/jp400718t  
**Kinetics and Physicochemical Process of Photoinduced Hydrophobic ↔ Superhydrophilic Switching of Pristine and N-doped TiO<sub>2</sub> Nanotube Arrays**  
Rajini P. Antony, Tom Mathews,\* S. Dash, and A. K. Tyagi

**6861** dx.doi.org/10.1021/jp400778k  
**Controlled Preparation of Uniform TiO<sub>2</sub>-Catalyzed Silver Nanoparticle Films for Surface-Enhanced Raman Scattering**  
Dawei Li, Lujun Pan,\* Shuai Li, Kun Liu, Shifa Wu, and Wei Peng

**6872**  dx.doi.org/10.1021/jp4009674  
**Investigation of Structural and Magnetic Properties of CoPt/CoAu Bimetallic Nanochains by X-ray Absorption Spectroscopy**  
Wei-Feng Huang, Qian Zhang, Dong-Feng Zhang, Jing Zhou, Cheng Si, Lin Guo,\* Wang-Sheng Chu,\* and Zi-Yu Wu\*

**6880**  dx.doi.org/10.1021/jp401305g  
**Experimental Characterization and Theoretical Modeling of a Linear [Co<sup>II</sup>,Tb<sup>III</sup>] Single Molecule Magnet**  
Oleg Reu, Andrei Palii, Serghei Ostrovsky, Warren Wallace, Oksana Zaharko,\* Vadapalli Chandrasekhar, Rodolphe Clerac, and Sophia Klokishner\*

**6889**  dx.doi.org/10.1021/jp401359a  
**Excited-State Absorption of Conjugated Polymers in the Near-Infrared and Visible: A Computational Study of Oligofluorenes**  
Sanliang Ling, Stefan Schumacher, Ian Galbraith, and Martin J. Paterson\*

**6896** dx.doi.org/10.1021/jp401423z  
**Thermal Stability and Shape Evolution of Tetrahedral Au–Pd Core–Shell Nanoparticles with High-Index Facets**  
Rao Huang, Yu-Hua Wen,\* Gui-Fang Shao, Zi-Zhong Zhu, and Shi-Gang Sun

**6904**  dx.doi.org/10.1021/jp402341w  
**Understanding the Control of Mineralization by Polyelectrolyte Additives: Simulation of Preferential Binding to Calcite Surfaces**  
Jia-Wei Shen, Chunli Li, Nico F. A. van der Vegt, and Christine Peter\*

## Comments

**6914** dx.doi.org/10.1021/jp312595p  
**Comment on “Using Photoelectron Spectroscopy and Quantum Mechanics to Determine d-Band Energies of Metals for Catalytic Applications”**  
Frank Abild-Pedersen, Anders Nilsson, and Jens K. Nørskov\*

**6916** dx.doi.org/10.1021/jp401620e  
**Reply to “Comment on ‘Using Photoelectron Spectroscopy and Quantum Mechanics to Determine d-Band Energies of Metals for Catalytic Applications’”**  
Timo Hofmann,\* Ted H. Yu, Michael Folse, Lothar Weinhardt, Marcus Bär, Yufeng Zhang, Boris V. Merinov, Deborah J. Myers, William A. Goddard III, and Clemens Heske\*

## Additions and Corrections

**6918** dx.doi.org/10.1021/jp400576j  
**Correction to “Luminescent Studies of “Exciplex Tuning” for Nanoclusters of Dicyanocuprate(I) Ions Doped in Potassium Chloride Crystals”**  
Haiyan Lu, Renante Yson, Xiaobo Li, Christie Larochele, and Howard H. Patterson\*

 Supporting Information available via online article