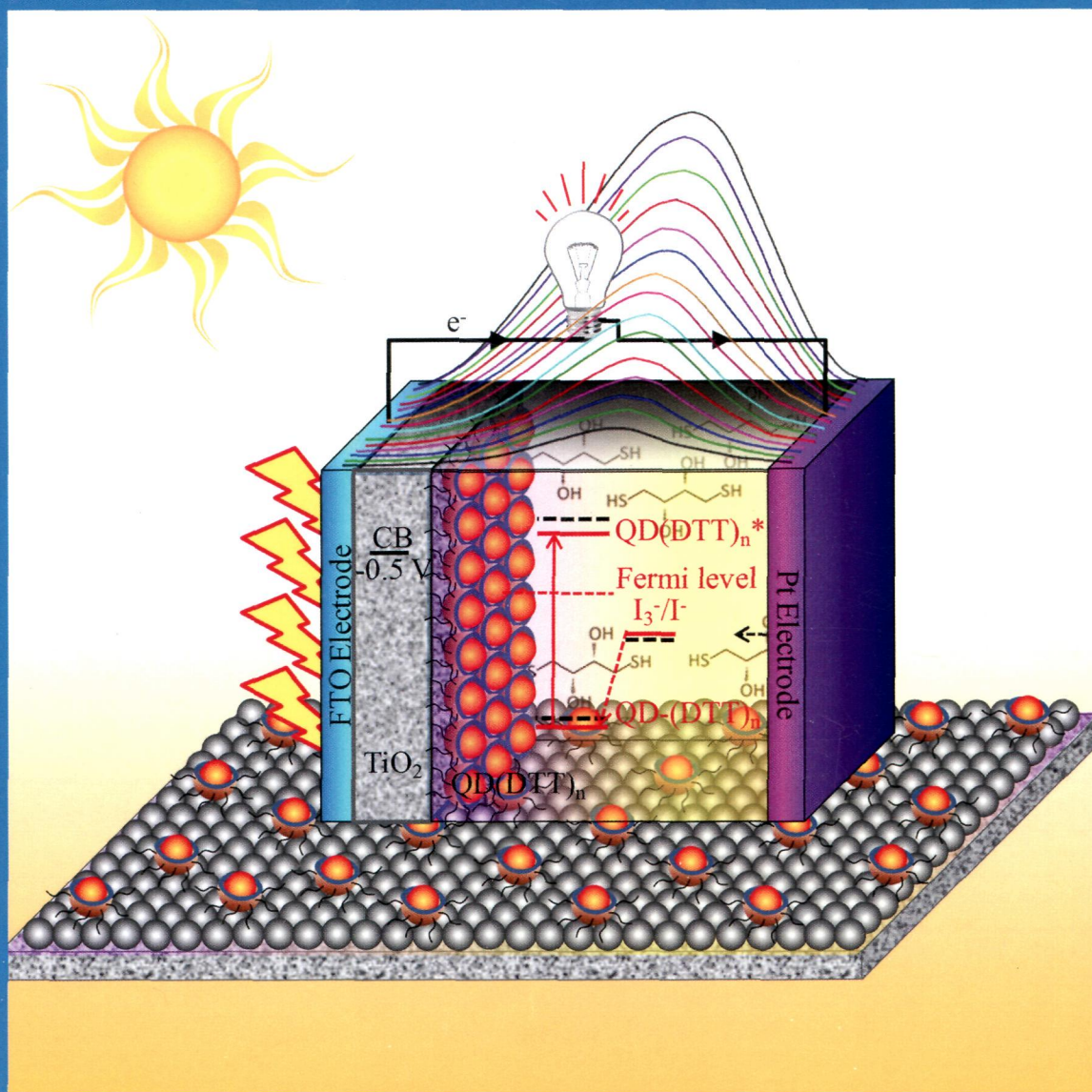


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C



Draining out the
 Last Electron:
 Photochemistry
 Helps out
 Solar Cell Technology
 (see page 5A)

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



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ON THE COVER: Draining out the last electron: photochemistry helps out solar cell technology. In situ passivation of defects in semiconductor quantum dots by simple thiol molecules enables us to classify and wipe out the centers of energy-wasting nonradiative carrier recombination. This defect-passivation helps us to improve the photoluminescence quantum efficiency of quantum-dot solutions, suppress the blinking of single quantum dots, and construct a quantum-dot-sensitized photoelectrochemical solar cell with higher photocurrent efficiency. See page 2178.

Articles

1755

[dx.doi.org/10.1021/jp310149y](https://doi.org/10.1021/jp310149y)

QM/MM Study of Photoinduced Reduction of a Tetrahedral Ag_{20}^+ Cluster by a Ag Atom

Hanning Chen,* Mark A. Ratner, and George C. Schatz*

Energy Conversion and Storage; Energy and Charge Transport

1763

[dx.doi.org/10.1021/jp4077245](https://doi.org/10.1021/jp4077245)

Possible Piezoelectric Materials $\text{CsMzr}_{0.5}(\text{MoO}_4)_3$ ($M = \text{Al}, \text{Sc}, \text{V}, \text{Cr}, \text{Fe}, \text{Ga}, \text{In}$) and $\text{CsCrTi}_{0.5}(\text{MoO}_4)_3$: Structure and Physical Properties

A. E. Sarapulova, B. Bazarov, T. Namsaraeva, S. Dorzhieva, J. Bazarova, V. Grossman, A. A. Bush, I. Antonyshyn, M. Schmidt, A. M. T. Bell, M. Knapp, H. Ehrenberg, J. Eckert, and D. Mikhailova*

1774

[dx.doi.org/10.1021/jp409634x](https://doi.org/10.1021/jp409634x)

Liquid Phase Deposition of Barium Hexaferrite Thin Films

Amin Yourdkhani, Daniela Caruntu, Armando K. Perez, and Gabriel Caruntu*

1783



[dx.doi.org/10.1021/jp409739b](https://doi.org/10.1021/jp409739b)

Spin-State Effects on the Thermal Dihydrogen Release from Solid-State $[\text{MH}(\eta^2\text{-H}_2)\text{dppe}_2]^+$ ($M = \text{Fe}, \text{Ru}, \text{Os}$) Organometallic Complexes for Hydrogen Storage Applications

David G. Abrecht, Jorge A. Muñoz, Hillary L. Smith, and Brent Fultz*

1793



[dx.doi.org/10.1021/jp410362d](https://doi.org/10.1021/jp410362d)

Effect of Substituents on Optical Properties and Charge-Carrier Polarity of Squaraine Dyes

Andrea M. Della Pelle, Paul J. Hornick, Youngju Bae, Paul M. Lahti,* and S. Thayumanavan*

1800  dx.doi.org/10.1021/jp410385s

Functionalized N-Doped Porous Carbon Nanofiber Webs for a Lithium–Sulfur Battery with High Capacity and Rate Performance

Juan Yang, Jing Xie, Xiangyang Zhou,* Youlan Zou, Jingjing Tang, Songcan Wang, Feng Chen, and Luyu Wang

1808  dx.doi.org/10.1021/jp410436f

Slow Charge Recombination and Enhanced Photoelectrochemical Properties of Diazaporphyrin-Fullerene Linked Dyad

Masanori Yamamoto, Yuta Takano, Yoshihiro Matano, Kati Stranius, Nikolai V. Tkachenko,* Helge Lemmetyinen, and Hiroshi Imahori*

1821 dx.doi.org/10.1021/jp410495k

Observation of Annealing-Induced Doping in TiO₂ Mesoporous Single Crystals for Use in Solid State Dye Sensitized Solar Cells

Varun Sivaram, Edward J. W. Crossland, Tomas Leijtens, Nakita K. Noel, Jack Alexander-Webber, Pablo Docampo, and Henry J. Snaith*

1828 dx.doi.org/10.1021/jp410510x

Conductivity and Wettability Changes of Ultrathin Nafion Films Subjected to Thermal Annealing and Liquid Water Exposure

Devproshad K. Paul and Kunal Karan*

1836 dx.doi.org/10.1021/jp410536n

Size Dependent Surface Charge Properties of Silica Nanoparticles

Murat Barisik, Selcuk Atalay, Ali Beskok, and Shizhi Qian*

1843  dx.doi.org/10.1021/jp410562u

Theoretical Prediction of the Rate Constants for Exciton Dissociation and Charge Recombination to a Triplet State in PCPDTBT with Different Fullerene Derivatives

Can Leng, Haimei Qin, Yubing Si, and Yi Zhao*

1856  dx.doi.org/10.1021/jp410644j

Estimating Hybridization of Transition Metal and Oxygen States in Perovskites from O K-edge X-ray Absorption Spectroscopy

Jin Suntivich,* Wesley T. Hong, Yueh-Lin Lee, James M. Rondinelli, Wanli Yang, John B. Goodenough, Bogdan Dabrowski, John W. Freeland, and Yang Shao-Horn*

1864 dx.doi.org/10.1021/jp411302d

One-Dimensional Single-Chain Molecular Magnet with a Cross-Linked π – π Coordination Network $\{[Co^II(\Delta)Co^III(A)](ox)_2(phen)_2\}_n$

Pramod Bhatt,* Nidhi Thakur, M. D. Mukadam, Sher Singh Meena, and S. M. Yusuf

Surfaces, Interfaces, Porous Materials, and Catalysis

1873  dx.doi.org/10.1021/jp4062016

Upright or Flat Orientations of the Ethanol Molecules on a Surface with Charge Dipoles and the Implication for Wetting Behavior

Chunlei Wang,* Liang Zhao, Donghua Zhang, Jige Chen, Guosheng Shi, and Haiping Fang

1879  dx.doi.org/10.1021/jp406688c

4,4'-Diaminodiphenyl Sulfone Functionalized SBA-15: Toluene Sensing Properties and Improved Proton Conductivity

Nana Qian, Zhiming Duan,* Yongheng Zhu, Qun Xiang, and Jiaqiang Xu*

1887  dx.doi.org/10.1021/jp407411k

Silicon Monomer Formation and Surface Patterning of Si(001)-2 \times 1 Following Tetraethoxysilane Dissociative Adsorption at Room Temperature

H eloise Tissot, Jean-Jacques Gallet,* Fabrice Bourmel, Ahmed Naitabdi, Debora Pierucci, Federica Bondino, Elena Magnano, Fran ois Rochet, and Fabio Finocchi

1894 dx.doi.org/10.1021/jp4082849

Atomic-Level Understanding of Interfaces in the Synthesis of Crystalline Oxides on Semiconductors: Sr- and Ba/Si(100)(2 \times 3) Reconstructions

Mikhail Kuzmin,* Marko P. J. Punkkinen, Pekka Laukkanen, Jouko J. K. L ang, Johnny Dahl, Levente Vitos, and Kalevi Kokko

1903  dx.doi.org/10.1021/jp4083823

Designing Thin Film-Capped Metallic Nanoparticles Configurations for Sensing Applications

Muhammad Y. Bashouti,* Adi-Solomon de la Zerda, Dolev Geva, and Hossam Haick

1910 dx.doi.org/10.1021/jp408444j

Ultrasonic Induced Rapid Formation and Crystal Refinement of Chemical Converted Hopeite Coating on Titanium

Xing-chuan Zhao, Gui-yong Xiao, Xian Zhang, Hong-yuan Wang, and Yu-peng Lu*

1919 dx.doi.org/10.1021/jp408866e





Electric-Field-Induced Second-Harmonic Generation Demonstrates Different Interface Properties of Molecular Beam Epitaxy Grown MgO on Si






Maarten K. Vanbel,* Chen-Yi Su, Jean-Pierre Locquet, and Thierry Verbiest

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Influence of the CO Adsorption Environment on Its Reactivity with (111) Terrace Sites in Stepped Pt Electrodes under Alkaline Media


Manuel J. S. Farias, Carlos Bus o-Rogero, Rub en Gisbert, Enrique Herrero,* and Juan M. Feliu*


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In Situ Characterizations of Nanostructured SnO₂/Pt(111) Surfaces Using Ambient-Pressure XPS (APXPS) and High-Pressure Scanning Tunneling Microscopy (HPSTM)
Stephanus Axnanda,* Zhongwei Zhu, Weiping Zhou, Baohua Mao, Rui Chang, Sana Rani, Ethan Crumlin, Gabor Somorjai, and Zhi Liu*
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Theoretical Study of the Energetic Stability and Geometry of Terminated and B-Doped Diamond (111) Surfaces
Shuainan Zhao* and Karin Larsson
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Catalytic Dissociation of Water on the (001), (011), and (111) Surfaces of Violarite, FeNi₂S₄: A DFT-D2 Study
Saima Haider, Alberto Roldan, and Nora H. de Leeuw*
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Nondestructive Monitoring of Defect Evolution in Epitaxial CdTe Thin Layers Grown on Si(111)
J. M. Oliveira, A. Malachias, C. A. Ospina, and S. O. Ferreira*
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Electronic and Geometric Structure of Ce³⁺ Forming Under Reducing Conditions in Shaped Ceria Nanoparticles Promoted by Platinum
O. V. Safonova,* A. A. Guda, C. Paun, N. Smolentsev, P. M. Abdala, G. Smolentsev, M. Nachttegaal, J. Szlachetko, M. A. Soldatov, A. V. Soldatov, and J. A. van Bokhoven*
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Ligand Dynamics of Drug-Loaded Microporous Zirconium Terephthalates-Based Metal–Organic Frameworks: Impact of the Nature and Concentration of the Guest
Sabine Devautour-Vinot,* Sekou Diaby, Denise da Cunha, Christian Serre, Patricia Horcajada, and Guillaume Maurin
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Hsuan Kung and Andrew V. Teplyakov*
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Characterization of Fe Substitution into La-Hexaaluminate Systems and the Effect on N₂O Catalytic Decomposition
Yan Zhang, Xiaodong Wang,* Yanyan Zhu, Baolin Hou, Xiaofeng Yang, Xin Liu, Junhu Wang, Jun Li, and Tao Zhang
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Nika Spiridis,* Ewa Madej, and Józef Korecki

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Critical Water Effect on the Plasmon Band and Visible Light Activity of Au/ZnO Nanocomposites
Matias E. Aguirre, G. Custo, Marcio S. Goes, Paulo R. Bueno, G. Zampieri, and Maria A. Grela*
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Adsorption and Photocatalytic Degradation of 3-Fluoroaniline on Anatase TiO₂(101): A Photoemission and Near-Edge X-ray Absorption Fine Structure Study
Mark J. Jackman and Andrew G. Thomas*
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Computer Screening of Dopants for the Development of New SnO₂-Based Transparent Conducting Oxides
Daojian Cheng, Minming Zhang, Jianfeng Chen,* Chenxi Yang, Xiaofei Zeng,* and Dapeng Cao
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Etching Silicon with HF-H₂O₂-Based Mixtures: Reactivity Studies and Surface Investigations
Christoph Gondek, Marcus Lippold, Ingo Röver, Klaus Bohmhammel, and Edwin Kroke*
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Superoleophobic Meshes with High Adhesion by Electrodeposition of Conducting Polymer Containing Short Perfluorobutyl Chains
Thierry Darmanin, Jeanne Tarrade, Elena Celia, and Frédéric Guittard*
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Understanding the Interface of Liquids with an Organic Crystal Surface from Atomistic Simulations and AFM Experiments
Peter Spijker,* Takumi Hiasa, Tiziana Musso, Rina Nishioka, Hiroshi Onishi, and Adam S. Foster
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New Insight into the Decomposition Mechanism of Formic Acid on Pd(111): Competing Formation of CO₂ and CO
Yingying Wang, Yuanyuan Qi, Dongju Zhang,* and Chengbu Liu
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Raman Enhancement of a Dipolar Molecule on Graphene
Changshui Huang, Myungwoong Kim, Bryan M. Wong, Nathaniel S. Safron, Michael S. Arnold, and Padma Gopalan*
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Time-of-Flight Secondary Ion Mass Spectrometry Investigation of the Orientation of Adsorbed Antibodies on SAMs Correlated to Biorecognition Tests
V. Lebec, S. Boujday, C. Poleunis, C.-M. Pradier, and A. Delcorte*

2093  dx.doi.org/10.1021/jp410910r
Assessing the Effects of Crowding, Pore Size, and Interactions on Electro-Osmotic Drag Coefficients
Liam C. Jacobson, Xiaoming Ren, and Valeria Molinero*

2104  dx.doi.org/10.1021/jp411051z
Coverage-Dependent Luminescence from Two-Dimensional Systems of Covalently Attached Perylene Fluorophores on Silica
Joseph M. McCrate and John G. Ekerdt*

2175  dx.doi.org/10.1021/jp4110695
Interaction of Hydrated Cations with Mica-*n* (*n* = 2, 3 and 4) Surface
Esperanza Pavón,* Miguel A. Castro, Agustín Cota, Francisco J. Osuna, M. Carolina Pazos, and Maria D. Alba

2122  dx.doi.org/10.1021/jp411183h
Single Layer of Polymeric Metal–Phthalocyanine: Promising Substrate to Realize Single Pt Atom Catalyst with Uniform Distribution
X. F. Chen, J. M. Yan, and Q. Jiang*


2129  dx.doi.org/10.1021/jp411299e
Interactions of Hydrogen and Carbon Monoxide on Pd–Au Bimetallic Surfaces
Wen-Yueh Yu, Gregory M. Mullen, and C. Buddie Mullins*


Plasmonics, Optical Materials, and Hard Matter

2138 dx.doi.org/10.1021/jp4110823
Plasmonic Fluorescence Enhancement of DBMBF₂ Monomers and DBMBF₂–Toluene Exciplexes using Al-Hole Arrays
Thomas M. Schmidt, Vladimir E. Bochenkov, Juan Diego A. Espinoza, Edsger C. P. Smits, Aziz M. Muzafarov, Yuriy N. Kononovich, and Duncan S. Sutherland*

2146 dx.doi.org/10.1021/jp411199r
Absorption of Water in Thermally Modified Pine Wood As Studied by Nuclear Magnetic Resonance
Päivi M. Kekkonen, Aapo Ylisassi, and Ville-Veikko Telkki*

Physical Processes in Nanomaterials and Nanostructures

2154  dx.doi.org/10.1021/jp4062303
Solution-Processed Small Molecule Donor/Acceptor Blends for Electrical Memory Devices with Fine-Tunable Storage Performance
Shifeng Miao, Yongxiang Zhu, Qing Bao, Hua Li, Najun Li, Shunjun Ji, Qingfeng Xu, Jianmei Lu,* and Lihua Wang

2161  dx.doi.org/10.1021/jp407388h
Decoration of WS₂ Nanotubes and Fullerene-Like MoS₂ with Gold Nanoparticles
Alexander Yu. Polyakov, Lena Yadgarov, Ronit Popovitz-Biro, Vasily A. Lebedev, Iddo Pinkas, Rita Rosentsveig, Yishay Feldman, Anastasia E. Goldt, Eugene A. Goodilin,* and Reshef Tenne

2170  dx.doi.org/10.1021/jp407940z
Carbon Dioxide Capture and Gas Separation on B₆₀ Fullerene
Qiao Sun,* Meng Wang, Zhen Li,* Aijun Du, and Debra J. Searles*

2178 dx.doi.org/10.1021/jp4083882
In Situ Photochemical Surface Passivation of CdSe/ZnS Quantum Dots for Quantitative Light Emission and Enhanced Photocurrent Response in Solar Cells
Morihiro Hamada, Norifumi Takenokoshi, Keiji Matozaki, Qi Feng, Norio Murase, Shin-ichi Wakida, Shunsuke Nakanishi, and Vasudevanpillai Biju*


2187 dx.doi.org/10.1021/jp409501g
Noncovalent Interaction with Graphene Oxide: The Crucial Role of Oxidative Debris
Vitor R. Coluci,* Diego Stéfani T. Martinez, Jaqueline G. Honório, Andréia F. de Faria, Daniel A. Moraes, Munir S. Skaf, Oswaldo L. Alves, and Gisela A. Umbuzeiro

2194 dx.doi.org/10.1021/jp4099599
Formation of Highly Ordered Organic Molecular Thin Films on Deactivated Si Surfaces Studied by Scanning Tunneling Microscopy and Low Energy Electron Diffraction
Sean R. Wagner and Pengpeng Zhang*

2202 dx.doi.org/10.1021/jp4100685
Blinking Statistics and Excitation-Dependent Luminescence Yield in Si and CdSe Nanocrystals
Benjamin Bruhn, Fatjon Qejvanaj, Ilya Sychugov,* and Jan Linnros

2209  dx.doi.org/10.1021/jp4102288
Mechanics and Energetics of DNA Hybridization on Single-Walled Carbon Nanotubes Explored Using Adaptive Biasing Force Calculations
Michael W. Chien, Robert R. Johnson, Shreekumar R. Pillai,* Shree Ram Singh, and A. T. Charlie Johnson Jr.*

2215  dx.doi.org/10.1021/jp410808z
Photoinduced Energy and Electron Transfer in Micellar Multilayer Films
Maciej Kopeć, Wiktor Niemiec, Andre Laschewsky, Maria Nowakowska,* and Szczepan Zapotoczny*

2222  dx.doi.org/10.1021/jp410813z
Synthesis of Crystalline Pyramidal ϵ -FeSi and Morphology- and Size-Dependent Ferromagnetism
Xiang Wang, Zhiqiang He, Shijie Xiong, and Xinglong Wu*

Effect of Polymer Chain Folding on the Transition from H- to J-Aggregate Behavior in P3HT Nanofibers

Mina Baghgar, Joelle A. Labastide, Felicia Bokel, Ryan C. Hayward, and Michael D. Barnes*

Additions and Corrections

2236

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Correction to "Azimuthal Dichroism in Near-Edge X-ray Absorption Fine Structure Spectra of Planar Molecules"

Guido Fratesi,* Valeria Lanzilotto, Luca Floreano, and Gian Paolo Brivio