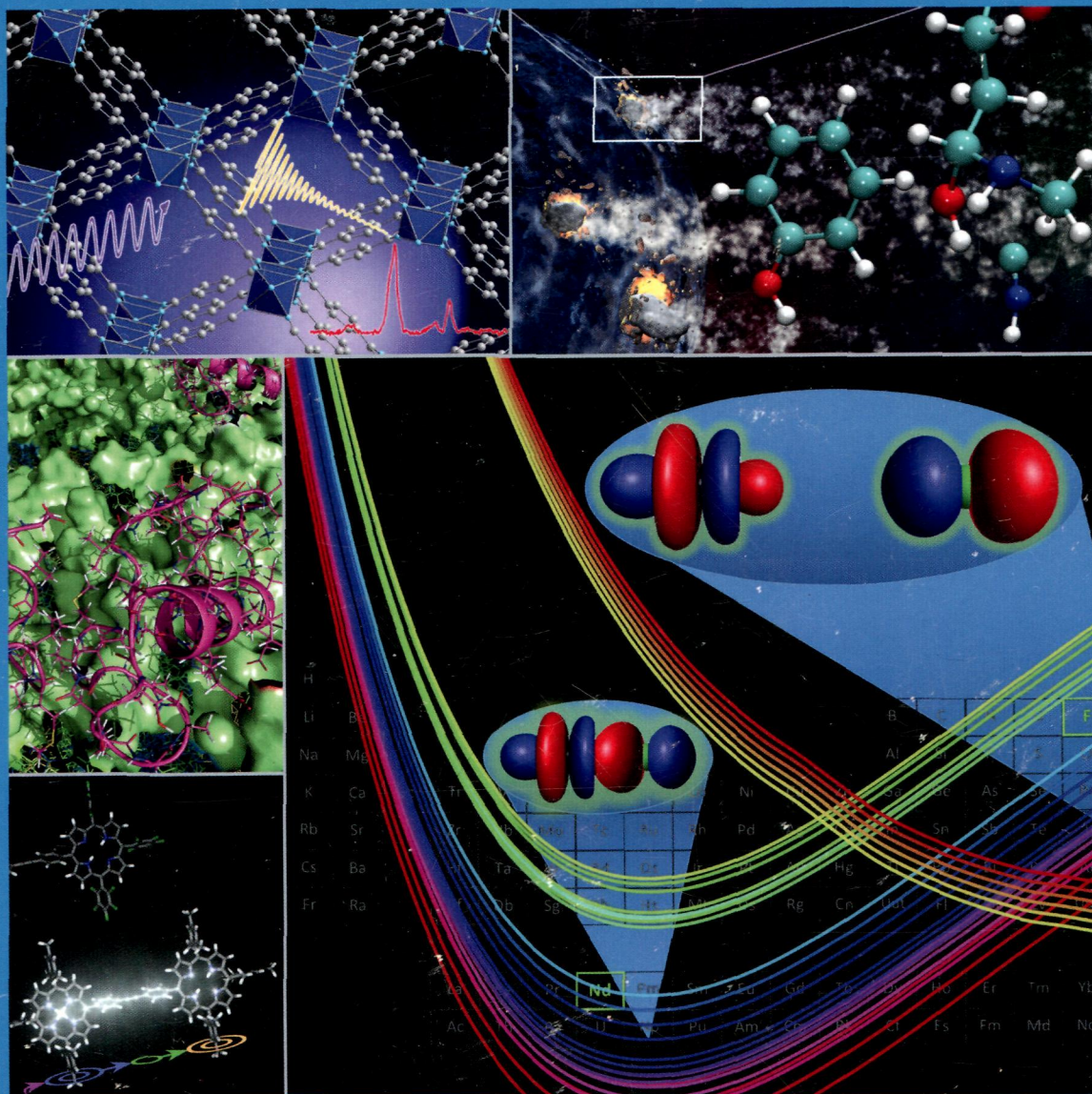


FEBRUARY 6, 2014
VOLUME 118
NUMBER 5
pubs.acs.org/JPCC

THE JOURNAL OF PHYSICAL CHEMISTRY

C



**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: Collage of cover art from recent issues of *J. Phys. Chem.* Top Left: ^{17}O Solid-State NMR Spectra Provide Signatures of Various Oxygen Species in Metal-Organic Frameworks (*J. Phys. Chem. C* **2013**, *117* (33), 16953–16960). Center Left: Behavior of Amyloid β -Peptides on a Ganglioside-Containing Membrane Surface (*J. Phys. Chem. B* **2013**, *117* (27), 8085–8094). Bottom Left: Bridge-Mediated EET in Porphyrin Dimers: Electronic Coupling Reduced by Fluorination (*J. Phys. Chem. C* **2013**, *117* (24), 12423–12431). Top Right: Synthesis of Prebiotic Hydrocarbons in Impacts of Simple Icy Mixtures on Early Earth (*J. Phys. Chem. A* **2013**, *117* (24), S124–S131). Bottom Right: Computed Potential Energy Curves for Quartet, Doublet, and Sextet States of NdF^{2+} (*J. Phys. Chem. A* **2013**, *117* (42), 10881–10888).

Articles

Energy Conversion and Storage; Energy and Charge Transport

2237



[dx.doi.org/10.1021/jp405744d](https://doi.org/10.1021/jp405744d)

Correlation between Polymer Structure and Polymer:Fullerene Blend Morphology and Its Implications for High Performance Polymer Solar Cells

Seon Kyoung Son, Youn-Su Kim, Hae Jung Son, Min Jae Ko, Honggon Kim, Doh-Kwon Lee, Jin Young Kim, Dong Hoon Choi, Kyungkon Kim,* and BongSoo Kim*

2245

[dx.doi.org/10.1021/jp4073284](https://doi.org/10.1021/jp4073284)

Effects of Current-Induced Forces on Pt–Benzene–Pt Single-Molecule Junctions

Bailey C. Hsu, Ilias Amanatidis, Wei-Lin Liu, Allen Tseng, and Yu-Chang Chen*

2253



[dx.doi.org/10.1021/jp408012d](https://doi.org/10.1021/jp408012d)

Near-Monolayer Platinum Shell on Core–Shell Nanocatalysts for High-Performance Direct Methanol Fuel Cell

Jang-Jung Wang, Yu-Ting Liu, I-Li Chen, Yaw-Wen Yang, Tsung-Kuang Yeh, Chih Hao Lee, Chi-Chang Hu, Ten-Chin Wen, Tsan-Yao Chen,* and Tsang-Lang Lin*

2263



[dx.doi.org/10.1021/jp408021m](https://doi.org/10.1021/jp408021m)

Graphene-Wrapped Mesoporous Cobalt Oxide Hollow Spheres Anode for High-Rate and Long-Life Lithium Ion Batteries


Hongtao Sun, Xiang Sun, Tao Hu, Mingpeng Yu, Fengyuan Lu, and Jie Lian*

2273

[dx.doi.org/10.1021/jp408945j](https://doi.org/10.1021/jp408945j)

Theoretical Study of Li Migration in Lithium–Graphite Intercalation Compounds with Dispersion-Corrected DFT Methods


Sascha Thinius, Mazharul M. Islam,* Paul Heitjans, and Thomas Bredow


2281  dx.doi.org/10.1021/jp4094904
Influence of the Nickel Oxide Nanostructure Morphology on the Effectiveness of Reduced Graphene Oxide Coating in Supercapacitor Electrodes
Gyeonghee Lee, Yingwen Cheng, Chakrapani V. Varanasi, and Jie Liu*

2287  dx.doi.org/10.1021/jp409583q
Photocurrent Generation in Bulk vs Bilayer Devices: Quantum Treatment of Model Rubrene/7,7,8,8-Tetracyanoquinodimethane Heterojunctions for Organic Solar Cells
Rui M. Pinto*

2298  dx.doi.org/10.1021/jp4101637
Semi-Empirical Limiting Efficiency of Singlet-Fission-Capable Polyacene/Inorganic Hybrid Solar Cells
M. J. Y. Tayebjee,* A. Mahboubi Soufiani, and G. J. Conibeer


2306 dx.doi.org/10.1021/jp410242e
Hydrogen Evolution from Pt Nanoparticles Covered p-Type CdS:Cu Photocathode in Scavenger-Free Electrolyte
Qiang Huang, Quan Li, and Xudong Xiao*


2312  dx.doi.org/10.1021/jp410784v
Carbazole-Derived Group of Uniform Materials Based on Organic Salts: Solid State Fluorescent Analogues of Ionic Liquids for Potential Applications in Organic-Based Blue Light-Emitting Diodes
Noureen Siraj, Farhana Hasan, Susmita Das,* Lucy W. Kiruri, Karen E. Steege Gall, Gary A. Baker, and Isiah M. Warner*


2321  dx.doi.org/10.1021/jp4112469
Bisdonor–azaBODIPY–Fullerene Supramolecules: Syntheses, Characterization, and Light-Induced Electron-Transfer Studies
Venugopal Bandi, Mohamed E. El-Khouly, Kei Ohkubo, Vladimir N. Nesterov, Melvin E. Zandler, Shunichi Fukuzumi,* and Francis D'Souza*

2333  dx.doi.org/10.1021/jp411437f
Predicting New TiO₂ Phases with Low Band Gaps by a Multiobjective Global Optimization Approach
Hou-Zun Chen, Yue-Yu Zhang, Xingao Gong,* and Hongjun Xiang*


2338 dx.doi.org/10.1021/jp411464w
Grain Boundary Effect on Electrical Transport Properties of Graphene
Hengji Zhang, Geunsik Lee, Cheng Gong, Luigi Colombo, and Kyeongjae Cho*

2344  dx.doi.org/10.1021/jp411551v
NH₃ Mediated or Ion Migration Reaction: The Case Study on Halide–Amide System
Hujun Cao, Jianhui Wang, Yongshen Chua, Han Wang, Guotao Wu, Zhitao Xiong, Jieshan Qiu, and Ping Chen*

2350  dx.doi.org/10.1021/jp411710b
Spectroscopic and Quantum Chemical Study of the Ni(P^{Ph}₂N^{C₆H₄CH₂P(O)(OEt)₂)₂ Electrocatalyst for Hydrogen Production with Emphasis on the Ni^I Oxidation State}
Amélie Kochem,* Frank Neese, and Maurice van Gastel*


2361  dx.doi.org/10.1021/jp4118908
Phosphorimetric Characterization of Solution-Processed Polymeric Oxygen Barriers for the Encapsulation of Organic Electronics
Eduardo Aluicio-Sarduy, Aliaksandr Baidak, Georgios C. Vougioukalakis, and Panagiotis E. Keivanidis*

2370 dx.doi.org/10.1021/jp412099y
Enhancement of Electrochemical Hydrogen Insertion in N-Doped Highly Ordered Mesoporous Carbon
Dan Liu, Dong Zheng, Lili Wang, Deyu Qu,* Zhizhong Xie, Jiaheng Lei, Liping Guo, Bohua Deng, Liang Xiao, and Deyang Qu*

2375  dx.doi.org/10.1021/jp412107g
Rational Design of Dibenzothiophene-Based Host Materials for PHOLEDs
Shou-Cheng Dong, Lei Zhang, Jian Liang, Lin-Song Cui, Qian Li, Zuo-Quan Jiang,* and Liang-Sheng Liao*


2385  dx.doi.org/10.1021/jp412257g
Toward Tandem Photovoltaic Devices Employing Nanoarray Graphene-Based Sheets
Yongfu Zhu, Ning Zhao, Jianshe Lian, and Qing Jiang*

Surfaces, Interfaces, Porous Materials, and Catalysis

2391  dx.doi.org/10.1021/jp412135v
Charged Particles Modulate Local Ionic Concentrations and Cause Formation of Positive Peaks in Resistive-Pulse-Based Detection
Justin Menestrina, Crystal Yang, Matthew Schiel, Ivan Vlasiouk, and Zuzanna S. Siwy*

2399 dx.doi.org/10.1021/jp4052193
Morphology Changes of Co Catalyst Nanoparticles at the Onset of Fischer–Tropsch Synthesis
Kristin Høydalsvik, Jostein B. Fløystad, Alexey Voronov, Georg J. B. Voss, Morteza Esmaeili, Jan Kehres, Håvard Granlund, Ulla Vainio, Jens W. Andreasen, Magnus Rønning, and Dag W. Breiby*

2408  dx.doi.org/10.1021/jp406042c
Temperature-Responsive Thin Films from Cellulose Stearoyl Triester
Andreas Geissler, Elmar Bonaccorso, Lars-Oliver Heim, Thomas Heinze, and Kai Zhang*








2418  dx.doi.org/10.1021/jp4063059
Structure of Normal-Alkanes Adsorbed on Hexagonal-Boron Nitride
Thomas Arnold,* Matthew Forster, Achilles Athanasiou Fragkoulis, and Julia E. Parker

- 2429 dx.doi.org/10.1021/jp406329n
Surface Chemistry and Atomic-Scale Reconstruction of Kerogen–Silica Composites
György Hantal,* Laurent Brochard, M. Natália Dias Soeiro Cordeiro, Franz J. Ulm, and Roland J.-M. Pellenq
- 2439 ⑤ dx.doi.org/10.1021/jp406610v
On the Promoting Effect of Water during NO_x Removal over Single-Site Copper in Hydrophobic Silica APD-Aerogels
Tina Kristiansen and Karina Mathisen*
- 2454 ⑤ dx.doi.org/10.1021/jp408354r
Influence of Silica Types on Synthesis and Performance of Amine–Silica Hybrid Materials Used for CO₂ Capture
Kai-Min Li, Jian-Guo Jiang,* Si-Cong Tian, Xue-Jing Chen, and Feng Yan
- 2463 dx.doi.org/10.1021/jp4087464
Tailoring the Electronic Band Gap of Graphyne
Jahyun Koo, Bing Huang, Hosik Lee, Gunn Kim, Jaewook Nam, Yongkyung Kwon, and Hoonkyung Lee*
- 2469 dx.doi.org/10.1021/jp409076y
The Roles of Reduced Ti Cations and Oxygen Vacancies in Water Adsorption and Dissociation on SrTiO₃(110)
Wentao Li, Shuming Liu, Shuai Wang, Qinlin Guo, and Jiandong Guo*
- 2475 dx.doi.org/10.1021/jp409385k
Langmuir–Hinshelwood Mechanism Including Lateral Interactions and Species Diffusion for CO Electro-Oxidation on Metallic Surfaces
Ana M. Gómez-Marín and Juan P. Hernández-Ortiz*
- 2487 ⑤ dx.doi.org/10.1021/jp409768j
Electronic Polarization at Pentacene/Polymer Dielectric Interfaces: Imaging Surface Potentials and Contact Potential Differences as a Function of Substrate Type, Growth Temperature, and Pentacene Microstructure
Yanfei Wu, Greg Haugstad, and C. Daniel Frisbie*
- 2498 ⑤ dx.doi.org/10.1021/jp409837d
Ab Initio Calculations of the Main Crystal Surfaces of Forsterite (Mg₂SiO₄): A Preliminary Study to Understand the Nature of Geochemical Processes at the Olivine Interface
M. Bruno,* F. R. Massaro, M. Prencipe, R. Demichelis, M. De La Pierre, and F. Nestola
- 2507 ⑤ dx.doi.org/10.1021/jp410198r
Integrated Synthesis of Nitrogen-Doped Mesoporous Carbon from Melamine Resins with Superior Performance in Supercapacitors
Meng Li and Junmin Xue*


- 2518 ⑤ dx.doi.org/10.1021/jp410255g
Effects of Substrate Molecular Structure on the Catalytic Activity of Peptide-Templated Pd Nanomaterials
Dennis B. Pacardo, Eric Ardman, and Marc R. Knecht*
- 2528 ⑤ dx.doi.org/10.1021/jp410790z
Water-Gas Shift Reaction on Ni–W–Ce Catalysts: Catalytic Activity and Structural Characterization
Fuzhen Zhao, Zongyuan Liu, Wenqian Xu, Siyu Yao, Anna Kubacka, Aaron C. Johnston-Peck, Sanjaya D. Senanayake, Ai-Qing Zhang, Eric A. Stach, Marcos Fernández-García, and José A. Rodríguez*
- 2539 dx.doi.org/10.1021/jp4108238
Electrochemical Impedance of Ion-Exchange Membranes in Ternary Solutions with Two Counterions
A. A. Moya
- 2554 ⑤ dx.doi.org/10.1021/jp4108766
H₂O/D₂O Exchange on SnO₂ Materials in the Presence of CO: Operando Spectroscopic and Electric Resistance Measurements
Roman G. Pavelko,* Joong-Ki Choi, Atsushi Urakawa, Masayoshi Yuasa, Tetsuya Kida, and Kengo Shimano
- 2564 dx.doi.org/10.1021/jp411083g
Adhesion-Regulated Switchable Fluid Slippage on Superhydrophobic Surfaces
Yang Wu, Yahui Xue, Xiaowei Pei, Meirong Cai, Huiling Duan,* Wilhelm T. S. Huck,* Feng Zhou,* and Qunji Xue
- 2570 ⑤ dx.doi.org/10.1021/jp411098y
Effect of N- α Substitution on the Electropolymerization of N-Substituted Pyrroles: Structure–Reactivity Relationship Studies
Sunil Kumar, Sada Krishnakanth, Jomon Mathew, Zvika Pomerantz, Jean-Paul Lellouche,* and Subrata Ghosh*
- 2580 dx.doi.org/10.1021/jp410652s
Predictive Morphology Control of Hydrogen-Terminated Silicon Nanoparticles
Hugh F. Wilson* and Amanda S. Barnard
- 2587 ⑤ dx.doi.org/10.1021/jp411241s
Stability and Composition of Helium Hydrates Based on Ices I_h and II at Low Temperatures
Rodion V. Belosludov,* Yulia Y. Bozhko, Oleg S. Subbotin, Vladimir R. Belosludov, Hiroshi Mizuseki, Yoshiyuki Kawazoe, and Vasily M. Fomin
- 2594 ⑤ dx.doi.org/10.1021/jp411442f
Size-Dependent Halogenated Nitrobenzene Hydrogenation Selectivity of Pd Nanoparticles
Jinghui Lyu, Jianguo Wang,* Chunshan Lu, Lei Ma, Qunfeng Zhang, Xiaobo He, and Xiaonian Li*

- 2602  dx.doi.org/10.1021/jp411637w
Reactive Landing of Dendrimer Ions onto Activated Self-Assembled Monolayer Surfaces
Qichi Hu and Julia Laskin*
- 2609  dx.doi.org/10.1021/jp4117134
Understanding Energy Transfer in Gas–Surface Collisions from Gas-Phase Models
Juan J. Nogueira, William L. Hase, and Emilio Martínez-Núñez*
- 2622  dx.doi.org/10.1021/jp4118584
Meta-Positioning of Carbonitrile Functional Groups Induces Interfacial Edge-On Phase of Oligophenyl Derivatives
Matthias Marschall, Joachim Reichert, Katharina Diller, Svetlana Klyatskaya, Mario Ruben, Alexei Nefedov, Christof Wöll, Lev N. Kantorovich, Florian Klappenberger,* and Johannes V. Barth
- 2634  dx.doi.org/10.1021/jp411871y
Particle-Size- and Ru-Core-Induced Surface Electronic States of Ru-Core/Pt-Shell Electrocatalyst Nanoparticles
Shuji Goto,* Shizuka Hosoi, Ryoji Arai, Shinji Tanaka, Minoru Umeda, Mamoru Yoshimoto, and Yoshihiro Kudo
- 2641 dx.doi.org/10.1021/jp411935g
Sidewall Chlorination of Carbon Nanotubes by Iodine Trichloride
Victor K. Abdelkader, María Domingo-García, M. Dolores Gutiérrez-Valero, Rafael López-Garzón, Manuel Melguizo, Celeste García-Gallarin, F. Javier Lopez-Garzon,* and Manuel J. Pérez-Mendoza
- 2650  dx.doi.org/10.1021/jp411979x
Electrochemical and Theoretical Study of π – π Stacking Interactions between Graphitic Surfaces and Pyrene Derivatives
Mengmei Cao, Aiping Fu, Zonghua Wang, Jingquan Liu,* Na Kong, Xidan Zong, Huihui Liu, and J. Justin Gooding*
- 2660   dx.doi.org/10.1021/jp412526t
Uncommon Synergy between Adsorption and Diffusion of Hexane Isomer Mixtures in MFI Zeolite Induced by Configurational Entropy Effects
Tobias Titze, Christian Chmelik, Jörg Kärger, Jasper M. van Baten, and Rajamani Krishna*
- 2666  dx.doi.org/10.1021/jp5001418
Predicting and Comparing C–M and O–M Bond Strengths for Adsorption on Transition Metal Surfaces
Matthew M. Montemore and J. Will Medlin*
- 2673 dx.doi.org/10.1021/jp500425g
Ion Adsorption on Modified Electrodes as Determined by Direct Force Measurements under Potentiostatic Control
Volodymyr Kuznetsov and Georg Papastavrou*


Plasmonics, Optical Materials, and Hard Matter

- 2686 dx.doi.org/10.1021/jp408901c
A New Blue-Emitting Oxohalide Phosphor $\text{Sr}_4\text{OCl}_6\text{:Eu}^{2+}$ for Thermally Stable, Efficient White-Light-Emitting Devices under Near-UV
Sun Joong Gwak, P. Arunkumar, and Won Bin Im*
- 2693  dx.doi.org/10.1021/jp412368m
Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations
Jihan Kim,* Li-Chiang Lin, Kyuho Lee, Jeffrey B. Neaton, and Berend Smit
- 2702  dx.doi.org/10.1021/jp410941t
In Situ Ultralow-Frequency Raman Tracking of the Polymorphic Transformation of Crystalline 1,1'-Binaphthyl
Chun-Fu Chang, Szu-Cheng Wang, and Shinsuke Shigeto*
- 2710  dx.doi.org/10.1021/jp412157c
Unified Theoretical Framework for Realizing Diverse Regimes of Strong Coupling between Plasmons and Electronic Transitions
Jacob A. Faucheaux, Jiayi Fu, and Prashant K. Jain*
- 2718  dx.doi.org/10.1021/jp412231w
Huge Energy Gain in Metal-to-Molecule Charge Transfer Processes: A Combined Effect of an Electrical Capacitive Enhancement in Nanometer-Size Hot Spots and the Electronic Structure of the Surface Complex
Jessica Roman-Perez, Cristina Ruano, Silvia P. Centeno, Isabel López-Tocón, Juan F. Arenas, Juan Soto,* and Juan C. Otero*
- Physical Processes in Nanomaterials and Nanostructures**
- 2726  dx.doi.org/10.1021/jp412148s
Effect of Surface Charge on the Resistive Pulse Waveshape during Particle Translocation through Glass Nanopores
Wen-Jie Lan, Clemens Kubeil, Jie-Wen Xiong, Andreas Bund, and Henry S. White*
- 2735  dx.doi.org/10.1021/jp406533u
Study of the Binding Interactions of a Hemicyanine Dye with Nanotubes of β -Cyclodextrin and Effect of a Hofmeister Series of Potassium Salts
M. Sowmiya, Amit K. Tiwari, Sonu, G. Eranna, Ashok K. Sharma, and Subit K. Saha*
- 2749  dx.doi.org/10.1021/jp409061g
Photoluminescence of Mid-Infrared HgTe Colloidal Quantum Dots
Sean Keuleyan, John Kohler, and Philippe Guyot-Sionnest*

- 2754  [dx.doi.org/10.1021/jp4096002](https://doi.org/10.1021/jp4096002)
Monoisomeric Phthalocyanines and Phthalocyanine–Fullerene Dyads with Polar Side Chains: Synthesis, Modeling, and Photovoltage
Jenni Ranta, Kimmo Kaunisto, Mika Niskanen, Alexander Efimov, Terttu I. Hukka, and Helge Lemmetyinen*
- 2766 [dx.doi.org/10.1021/jp409620w](https://doi.org/10.1021/jp409620w)
Synthesis and Characterization of the Nonlinear Optical Properties of Novel Hybrid Organic–Inorganic Semiconductor Lead Iodide Quantum Wells and Dots
I. Papagiannouli, E. Maratou, I. Koutselas,* and S. Couris*
- 2776  [dx.doi.org/10.1021/jp409653t](https://doi.org/10.1021/jp409653t)
Sorption of Gold by Naked and Thiol-Capped Magnetite Nanoparticles: An XPS Approach
O. F. Odio, L. Lartundo-Rojas, P. Santiago-Jacinto, R. Martínez, and E. Reguera*
- 2792  [dx.doi.org/10.1021/jp410030b](https://doi.org/10.1021/jp410030b)
Chemiluminescence as a Novel Indicator for Interactions of Surfactant–Polymer Mixtures at the Surface of Layered Double Hydroxides
Weijiang Guan, Wenjuan Zhou, Qianwen Huang, and Chao Lu*
- 2799 [dx.doi.org/10.1021/jp410108f](https://doi.org/10.1021/jp410108f)
Spin–Orbit Gaps in Carbynes
Pavel N. D'yachkov* and Vasilii A. Zaluev
- 2804 [dx.doi.org/10.1021/jp4101619](https://doi.org/10.1021/jp4101619)
Improved Oxygen Reduction Performance of Pt–Ni Nanoparticles by Adhesion on Nitrogen-Doped Graphene
Eduardo Gracia-Espino, Xueen Jia, and Thomas Wågberg*
- 2812 [dx.doi.org/10.1021/jp410638r](https://doi.org/10.1021/jp410638r)
Plasmon Enhanced Heterogeneous Electron Transfer: A Model Study
Luxia Wang* and Volkhard May*
- 2820  [dx.doi.org/10.1021/jp410993a](https://doi.org/10.1021/jp410993a)
Monochromatic Near-Infrared to Near-Infrared Upconversion Nanoparticles for High-Contrast Fluorescence Imaging
Jiayin Zhang, Hua Zhao, Xitian Zhang, Xuanzhang Wang, Hong Gao,* Zhiguo Zhang,* and Wenwu Cao*
- 2826 [dx.doi.org/10.1021/jp4110568](https://doi.org/10.1021/jp4110568)
Start-Up of Electrokinetic Flow in a Fibrous Porous Medium
Guan Y. Chen and Huan J. Keh*


- 2834  [dx.doi.org/10.1021/jp411176b](https://doi.org/10.1021/jp411176b)
Structural Changes in Reduced Graphene Oxide upon MnO₂ Deposition by the Redox Reaction between Carbon and Permanganate Ions
Suk-Woo Lee, Seong-Min Bak, Chang-Wook Lee, Cherno Jaye, Daniel A. Fischer, Bae-Kyun Kim, Xiao-Qing Yang, Kyung-Wan Nam,* and Kwang-Bum Kim*


- 2844 [dx.doi.org/10.1021/jp4112553](https://doi.org/10.1021/jp4112553)
Ultrafast Spectroscopy of CdSe Nanocrystals: Morphological and Environmental Effects on Nonradiative and Nonadiabatic Relaxation
Bryan T. Spann and Xianfan Xu*

- 2851  [dx.doi.org/10.1021/jp411290z](https://doi.org/10.1021/jp411290z)
Organo-Modified Montmorillonite Enhanced Chemiluminescence via Inactivation of Halide Counterions in a Micellar Solution
Shuang Chen, Wenjuan Zhou, Yuqing Cao, Congcong Xue, and Chao Lu*

- 2857 [dx.doi.org/10.1021/jp4115833](https://doi.org/10.1021/jp4115833)
Surface Effects Under Visible Irradiation and Heat Treatment on the Phase Stability of γ -Fe₂O₃ Nanoparticles and γ -Fe₂O₃–SiO₂ Core–Shell Nanostructures
Luigi Stagi, Jose A. De Toro, Andrea Ardu, Carla Cannas, Alberto Casu, Su Seong Lee, and Pier Carlo Ricci*

- 2867 [dx.doi.org/10.1021/jp411695m](https://doi.org/10.1021/jp411695m)
Harnessing the Shape-Induced Optical Anisotropy of a Semiconductor Nanocrystal: A New Type of Intraband Absorption Spectroscopy
Anvar S. Baimuratov, Ivan D. Rukhlenko,* Vadim K. Turkov, Mikhail Yu. Leonov, Alexander V. Baranov, Yurii K. Gun'ko, and Anatoly V. Fedorov

- 2877  [dx.doi.org/10.1021/jp411723m](https://doi.org/10.1021/jp411723m)
Electron Paramagnetic Resonance Investigation of Charge Transfer in TiO₂(B)/Anatase and N–TiO₂(B)/Anatase Mixed-Phase Nanowires: The Relative Valence and Conduction Band Edges in the Two Phases
Hsin-Hsi Lo, Neeruganti O. Gopal, Shiann-Cherng Sheu, and Shyue-Chu Ke*

- 2885  [dx.doi.org/10.1021/jp412497k](https://doi.org/10.1021/jp412497k)
Production Rate and Reactivity of Singlet Oxygen ¹O₂(¹Δ_g) Directly Photoactivated at 1270 nm in Lipid Nanocapsules Dispersed in Water
A. Sivéry, A. Barras, R. Boukherroub, C. Pierlot, J. M. Aubry, F. Anquez, and E. Courtade*

Comments

- 2894 [dx.doi.org/10.1021/jp500336g](https://doi.org/10.1021/jp500336g)
Comment on “Surface Acidity of Water Probed by Free Energy Calculation for Trimethylamine Protonation”
Agustín J. Colussi* and Shinichi Enami