

ПИ
780/pc2

JUNE 26, 2014

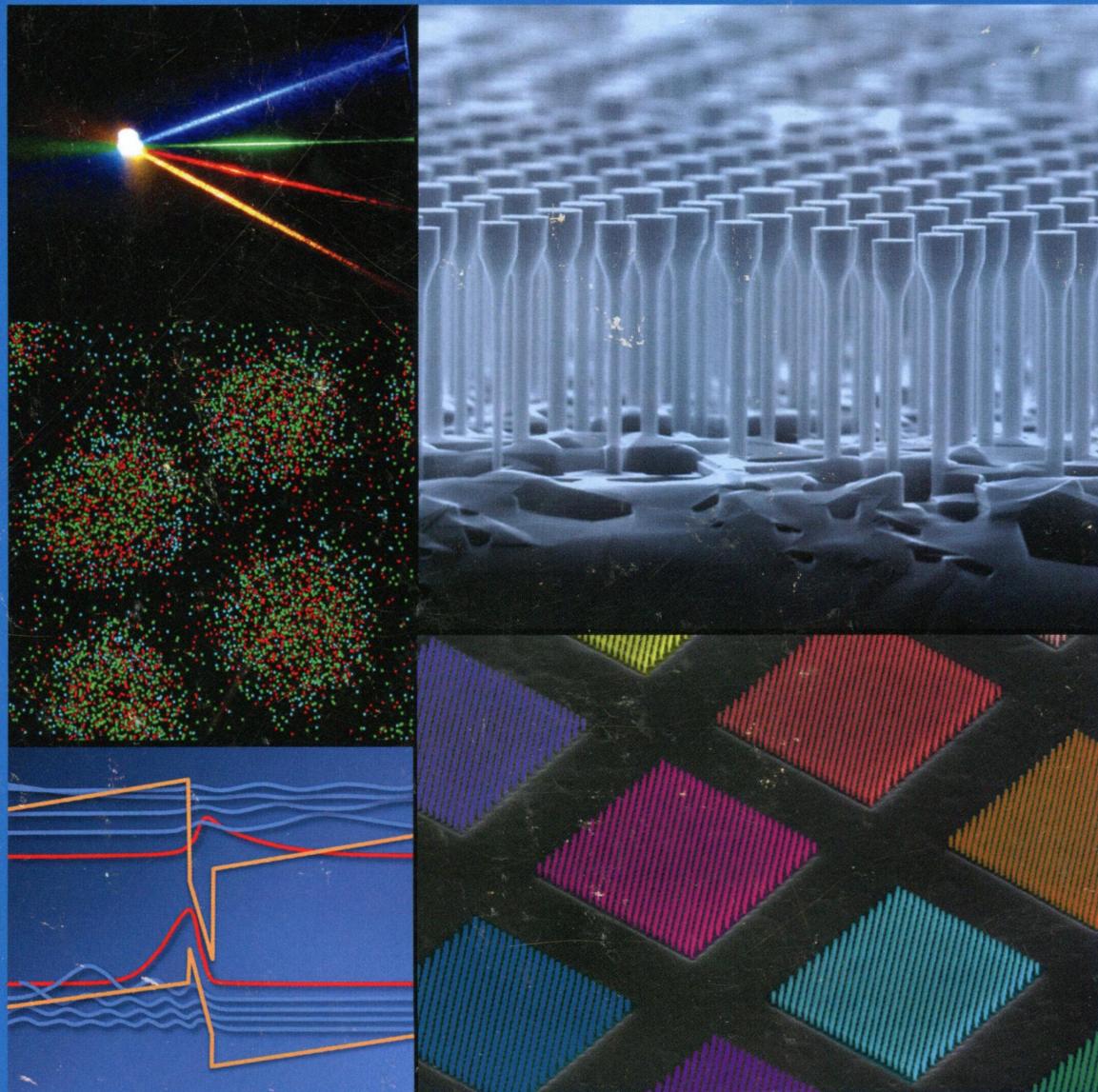
VOLUME 118

NUMBER 25

pubs.acs.org/JPCC

THE JOURNAL OF PHYSICAL CHEMISTRY C

Solid-State Lighting
Research: Exploring
Energy Conversion
in Tailored Photonic
Nanostructures
(see page 13330)



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



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

THE JOURNAL OF PHYSICAL CHEMISTRY C

JUNE 26, 2014

VOLUME 118 ISSUE 25

JPCCCK 118(25) 13329–14060 (2014)

ISSN 1932-7447

Registered in the U.S. Patent and Trademark Office

© 2014 by the American Chemical Society

ON THE COVER: Solid-state lighting research: exploring energy conversion in tailored photonic nanostructures. Research into emission phenomena that could lead to next-generation solid-state lighting. Images, clockwise from the upper left: emission from blue, green, red and amber lasers combined to produce white light (photo credit: Randy Montoya); array of GaN/InGaN nanowire light-emitting diode (LED) structures; false-color scanning electron microscope image of $10 \mu\text{m} \times 10 \mu\text{m}$ arrays of nanowire photonic-crystal laser structures, each with a different emission wavelength determined by nanowire diameter and spacing; electron and hole wave functions in a GaN/InGaN LED quantum-well structure; and elemental composition of CdSe/ZeSe quantum dots determined by transmission electron microscope energy-dispersive spectroscopy (Cd red, Se green, Zn blue). Cover art created by George Wang and Jeremy Wright. See page 13330.

Editorial

13329

[dx.doi.org/10.1021/jp503709n](https://doi.org/10.1021/jp503709n)

EFRC Feature Articles

Anne B. McCoy, Sharon Hammes-Schiffer, Catherine J. Murphy, and George C. Schatz*

Feature Article

13330

[dx.doi.org/10.1021/jp501136j](https://doi.org/10.1021/jp501136j)

Energy Frontier Research Center for Solid-State Lighting Science: Exploring New Materials Architectures and Light Emission Phenomena

Michael E. Coltrin,* Andrew M. Armstrong, Igal Brener, Weng W. Chow, Mary H. Crawford, Arthur J. Fischer, David F. Kelley, Daniel D. Koleske, Lincoln J. Lauhon, James E. Martin, May Nyman, E. Fred Schubert, Lauren E. Shea-Rohwer, Ganapathi Subramania, Jeffrey Y. Tsao, George T. Wang, Jonathan J. Wierer Jr., and Jeremy B. Wright

Articles

Energy Conversion and Storage; Energy and Charge Transport

13346

[dx.doi.org/10.1021/jp500352h](https://doi.org/10.1021/jp500352h)

First-Principles Study of Lanthanum Strontium Manganite: Insights into Electronic Structure and Oxygen Vacancy Formation

Michele Pavone, Ana B. Muñoz-García, Andrew M. Ritzmann, and Emily A. Carter*

13357

[dx.doi.org/10.1021/jp500371w](https://doi.org/10.1021/jp500371w)

Structure and Properties of Novel Cobalt-Free Oxides $\text{Nd}_x\text{Sr}_{1-x}\text{Fe}_{0.8}\text{Cu}_{0.2}\text{O}_{3-\delta}$ ($0.3 \leq x \leq 0.7$) as Cathodes of Intermediate Temperature Solid Oxide Fuel Cells

Jie-Wei Yin, Yi-Mei Yin,* Jun Lu, Chunming Zhang, Nguyen Q. Minh, and Zi-Feng Ma*

13369

[dx.doi.org/10.1021/jp5005117](https://doi.org/10.1021/jp5005117)

Confine Sulfur in Polyaniline-Decorated Hollow Carbon Nanofiber Hybrid Nanostructure for Lithium–Sulfur Batteries
Zhan Zhang,* Qiang Li, Yanqing Lai, and Jie Li

13377



[dx.doi.org/10.1021/jp500813r](https://doi.org/10.1021/jp500813r)

Cobalt-Bisglyoximato Diphenyl Complex as a Precatalyst for Electrocatalytic H₂ Evolution
Elodie Anxolabéhère-Mallart,* Cyrille Costentin,* Maxime Fournier, and Marc Robert*

13382

[dx.doi.org/10.1021/jp5012632](https://doi.org/10.1021/jp5012632)

Hierarchical Columnar RuO₂ Nanoplates and Their Improved Cycle Life Performance at High Capacity
Anantharamulu Navulla, Geoffrey Stevens, Igor Kovalenko, and Lamartine Meda*

13387

[dx.doi.org/10.1021/jp501531h](https://doi.org/10.1021/jp501531h)

High Field MAS NMR and Conductivity Study of the Superionic Conductor LiH₂PO₄: Critical Role of Physisorbed Water in Its Protonic Conductivity
Jin Jung Kweon, Riqiang Fu,* Eden Steven, Cheol Eui Lee, and Naresh S. Dalal*

13394

[dx.doi.org/10.1021/jp501892x](https://doi.org/10.1021/jp501892x)

Stripline ⁷⁵As NMR Study of Epitaxial III–V Semiconductor Al_{0.5}Ga_{0.5}As
M. Goswami, P. J. Knijn, G. J. Bauhuis, J. W. G. Janssen, P. J. M. van Bentum, G. A. de Wijs, and A. P. M. Kentgens*

13406

[dx.doi.org/10.1021/jp502319p](https://doi.org/10.1021/jp502319p)

In Silico Based Rank-Order Determination and Experiments on Nonaqueous Electrolytes for Sodium Ion Battery Applications

Ganesh Kamath, Richard W. Cutler, Sanket A. Deshmukh, Mehdi Shakourian-Fard, Riley Parrish, Joshua Huether, Darryl P. Butt, H. Xiong,* and Subramanian K. R. S. Sankaranarayanan*

13417



[dx.doi.org/10.1021/jp5024586](https://doi.org/10.1021/jp5024586)

Carrier Localization in Nanocrystalline Silicon

Luigi Bagolini, Alessandro Mattoni, Reuben T. Collins, and Mark T. Lusk*

13424

[dx.doi.org/10.1021/jp5028788](https://doi.org/10.1021/jp5028788)

Dynamic Characterization of Green-Sensitive Organic Photodetectors Using Nonfullerene Small Molecules: Frequency Response Based on the Molecular Structure

Kwang-Hee Lee, Gae Hwang Lee, Dong-Seok Leem, Jiyoul Lee, Jong Won Chung, Xavier Bulliard, Hyeonho Choi, Kyung-Bae Park, Kyu-Sik Kim, Yong Wan Jin,* Sangyoon Lee, and Soo Young Park*

13432

[dx.doi.org/10.1021/jp502910j](https://doi.org/10.1021/jp502910j)

Structure of Platinum Catalysts under CO, Hydrogen, and Oxygen; Anomalous Behavior of Pt on Ceria after Cyanide Leaching

Jeroen A. van Bokhoven,* Cristina Paun, and Jagdeep Singh

13444

Origin of Red Shift in the Photoabsorption Peak in MEH-PPV Polymer

Santanab Giri,* Corell H. Moore, James T. McLeskey, and Puru Jena

[dx.doi.org/10.1021/jp5030069](https://doi.org/10.1021/jp5030069)

13451

Lithium Borohydride Ethylenediamines: A Case Study of Solid-State LiBH₄-Organic Amine Complexes

Juner Chen, Teng He, Guotao Wu,* Zhitao Xiong, Lin Liu, Xiaohua Ju, and Ping Chen*

[dx.doi.org/10.1021/jp503123d](https://doi.org/10.1021/jp503123d)

13460

Impact of Acceptor Crystallinity on the Photophysics of Nonfullerene Blends for Organic Solar Cells

Paul E. Shaw,* Pascal Wolfer, Benjamin Langley, Paul L. Burn, and Paul Meredith

[dx.doi.org/10.1021/jp503150u](https://doi.org/10.1021/jp503150u)

13467

Facile and Scalable Synthesis of "Caterpillar-like" ZnO Nanostructures with Enhanced Photoelectrochemical Water-Splitting Effect

Qiang Li, Xing Sun, Karen Lozano, and Yuanbing Mao*

[dx.doi.org/10.1021/jp503155c](https://doi.org/10.1021/jp503155c)

13476

Pressure-Induced Conformational Change in Organic Semiconductors: Triggering a Reversible Phase Transition in Rubrene

Stefano Bergantin, Massimo Moret, Gernot Buth, and Francesca P. A. Fabbiani*

[dx.doi.org/10.1021/jp503271h](https://doi.org/10.1021/jp503271h)

13484

Influence of Oxygen Impurities on the Electrochromic Response of Viologen-Based Plastic Films

Giuseppe Chidichimo, Bruna Clara De Simone, Daniela Imbardelli, Maurizio De Benedictis, Marianna Barberio, Loredana Ricciardi, and Amerigo Beneduci*

[dx.doi.org/10.1021/jp503740u](https://doi.org/10.1021/jp503740u)

13493

Instantaneous Reduction of Graphene Oxide Paper for Supercapacitor Electrodes with Unimpeded Liquid Permeation

Zheng Bo,* Weiguang Zhu, Xin Tu, Yong Yang, Shun Mao, Yong He, Junhong Chen, Jianhua Yan, and Kefa Cen

[dx.doi.org/10.1021/jp5037734](https://doi.org/10.1021/jp5037734)

13503

Photoinduced Electron Transfer from a Tetrathiafulvalene-Calix[4]pyrrole to a Porphyrin Carboxylate within a Supramolecular Ensemble

Christina M. Davis, Yuki Kawashima, Kei Ohkubo, Jong Min Lim, Dongho Kim,* Shunichi Fukuzumi,* and Jonathan L. Sessler*

[dx.doi.org/10.1021/jp504087b](https://doi.org/10.1021/jp504087b)

13514

First-Principles Characterization of the *P2,ab* Ferroelectric Phase of Aurivillius Bi₂WO₆

Hania Djani,* Patrick Hermet, and Philippe Ghosez

[dx.doi.org/10.1021/jp504674k](https://doi.org/10.1021/jp504674k)

Surfaces, Interfaces, Porous Materials, and Catalysis

13525

[dx.doi.org/10.1021/jp4070328](https://doi.org/10.1021/jp4070328)

Tungsten Carbide Supports for Single-Atom Platinum-Based Fuel-Cell Catalysts: First-Principles Study on the Metal–Support Interactions and O₂ Dissociation on W_xC Low-Index Surfaces

Chee Kok Poh, San Hua Lim, Jianyi Lin, and Yuan Ping Feng*

13539

[dx.doi.org/10.1021/jp407275e](https://doi.org/10.1021/jp407275e)

Electronic Structure of Interfaces between Thiophene and TiO₂ Nanostructures

Marcelo Alves-Santos, Leonardo M. Marion Jorge,* Marilia J. Caldas,* and Daniele Varsano*

13545

[dx.doi.org/10.1021/jp412375z](https://doi.org/10.1021/jp412375z)

Fabrication of N-TiO₂/InBO₃ Heterostructures with Enhanced Visible Photocatalytic Performance

Yanlong Yu, Yue Tang, Jixiang Yuan, Qiang Wu, Wenjun Zheng,* and Yaan Cao*

13552

[dx.doi.org/10.1021/jp412662x](https://doi.org/10.1021/jp412662x)

Dewetting Dynamics of a Solid Microsphere by Emulsion Drops

Feng Lin, Lin He, Bauyrzhan Primkulov, and Zhenghe Xu*

13563

[dx.doi.org/10.1021/jp500472p](https://doi.org/10.1021/jp500472p)

Role of Electronegative Substituents on the Bond Energies in the Grubbs Metathesis Catalysts for M = Fe, Ru, Os

Monica Vasiliu, Anthony J. Arduengo III, and David A. Dixon*

13578

[dx.doi.org/10.1021/jp501318p](https://doi.org/10.1021/jp501318p)

Role of Surface Hydroxyl Groups on Zinc Adsorption Characteristics on α -Al₂O₃(0001) Surfaces: First-Principles Study

Rémi Cavallotti, Jacek Goniakowski,* Rémie Lazzari, Jacques Jupille, Alexey Koltsov, and Didier Loison

13590

[dx.doi.org/10.1021/jp5014362](https://doi.org/10.1021/jp5014362)

Effect of Porosity on the Infrared Radiative Properties of Plasma-Sprayed Yttria-Stabilized Zirconia Ceramic Thermal Barrier Coatings

Leire del Campo,* Domingos De Sousa Meneses, Karine Wittmann-Ténèze, Antoine Bacciochini, Alain Denoirjean, and Patrick Echegut

13598

[dx.doi.org/10.1021/jp501540y](https://doi.org/10.1021/jp501540y)

Molecular Reorientation and Structural Changes in Cosolvent-Treated Highly Conductive PEDOT:PSS Electrodes for Flexible Indium Tin Oxide-Free Organic Electronics

Claudia M. Palumbiny, Christoph Heller, Christoph J. Schaffer, Volker Körstgens, Gonzalo Santoro, Stephan V. Roth, and Peter Müller-Buschbaum*

13607

[dx.doi.org/10.1021/jp502031h](https://doi.org/10.1021/jp502031h)

First-Principles Investigation of Dehydrogenation on Cu-Doped MgH₂ (001) and (110) Surfaces

Hai-Chen Wang, Dong-Hai Wu, Liu-Ting Wei, and Bi-Yu Tang*

13617

[dx.doi.org/10.1021/jp502040y](https://doi.org/10.1021/jp502040y)

Catalyst Design Based on DFT Calculations: Metal Oxide Catalysts for Gas Phase NO Reduction
Xuesen Du, Xiang Gao,* Wenshuo Hu, Jinpin Yu, Zhongyang Luo, and Kefa Cen

13623

[dx.doi.org/10.1021/jp502106t](https://doi.org/10.1021/jp502106t)

Experimental Characterization of Unimolecular Water Dissociative Adsorption on α -Alumina
Harald Kirsch, Jonas Wirth, Yujin Tong, Martin Wolf, Peter Saalfrank, and R. Kramer Campen*

13631

[dx.doi.org/10.1021/jp5026619](https://doi.org/10.1021/jp5026619)

A Combined Ion Scattering, Photoemission, and DFT Investigation on the Termination Layer of a $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ Spin Injecting Electrode

L. Poggini, S. Ninova, P. Graziosi, M. Mannini,* V. Lanzilotto, B. Cortigiani, L. Malavolti, F. Borgatti, U. Bardi, F. Totti, I. Bergenti, V. A. Dedi, and R. Sessoli*

13638

[dx.doi.org/10.1021/jp502807z](https://doi.org/10.1021/jp502807z)

Self-Poisoning Dynamical Effects in the Oxygen Reduction Reaction on Pt(111) from a Top-Down Kinetic Analysis
Nicéphore Bonnet,* Minoru Otani, and Osamu Sugino

13644

[dx.doi.org/10.1021/jp502876r](https://doi.org/10.1021/jp502876r)

Electronic Structure and Optical Quality of Nanocrystalline Y_2O_3 Film Surfaces and Interfaces on Silicon
E. J. Rubio, V. V. Atuchin,* V. N. Kruchinin, L. D. Pokrovsky, I. P. Prosvirin, and C. V. Ramana

13652

[dx.doi.org/10.1021/jp503088h](https://doi.org/10.1021/jp503088h)

Novel Delta-Ta₂O₅ Structure Obtained from DFT Calculations
Z. Helali, M. Calatayud,* and C. Minot*

13659

[dx.doi.org/10.1021/jp503046w](https://doi.org/10.1021/jp503046w)

Self-Metalation of 2H-Tetraphenylporphyrin on Cu(111) Studied with XSW: Influence of the Central Metal Atom on the Adsorption Distance
C. Bürker, A. Franco-Cañellas, K. Broch, T.-L. Lee, A. Gerlach,* and F. Schreiber

13667

[dx.doi.org/10.1021/jp503269n](https://doi.org/10.1021/jp503269n)

Relative Stability of F-Covered TiO₂ Anatase (101) and (001) Surfaces from Periodic DFT Calculations and ab Initio Atomistic Thermodynamics
Oriol Lamiel-Garcia, Sergio Tosoni, and Francesc Illas*

13674

[dx.doi.org/10.1021/jp503402w](https://doi.org/10.1021/jp503402w)

Subsurface Charge Repulsion of Adsorbed H-Adatoms on TiO₂(110)
Jo Onoda, Chi Lun Pang,* Ayhan Yurtsever,* and Yoshiaki Sugimoto

13680

dx.doi.org/10.1021/jp503478c

IR Spectroscopic Behavior of Polaronic Trapped Electrons in TiO₂ under Aqueous Photocatalytic Conditions

David M. Savory and A. James McQuillan*

13693

dx.doi.org/10.1021/jp5035536

Luminescence Properties of Nitrogen-Doped ZnO

Fernando Stavale, Leandro Pascua, Niklas Nilius,* and Hans-Joachim Freund

13697

dx.doi.org/10.1021/jp503646u

Surface Dipoles and Electron Transfer at the Metal Oxide–Metal Interface: A 2PPE Study of Size-Selected Metal Oxide Clusters Supported on Cu(111)

Yixiong Yang, Jia Zhou, Miki Nakayama, Lizhou Nie, Ping Liu, and Michael G. White*

13707

dx.doi.org/10.1021/jp503853f

Quantifying the Impact of Relativity and of Dispersion Interactions on the Activation of Molecular Oxygen Promoted by Noble Metal Nanoparticles

Mohammed Benali Kanoun and Luigi Cavallo*

13715

dx.doi.org/10.1021/jp503916e

Effect of Modification with Vanadium or Carbon on Destructive Sorption of Halocarbons over Nanocrystalline MgO: The Role of Active Sites in Initiation of the Solid-State Reaction

Alexander F. Bedilov,* Ekaterina I. Shuvarkova, Alexander M. Volodin, Ekaterina V. Illyina, Ilya V. Mishakov, Aleksey A. Vedyagin, Vladimir V. Chesnokov, David S. Heroux, and Kenneth J. Klabunde

13726

dx.doi.org/10.1021/jp503966r

Surface Structural Reconstruction for Optical Response in Iodine-Modified TiO₂ Photocatalyst System

Linjuan Zhang, Jing Zhou, Jiong Li, Gang Liu, Xiao Lin, Baohua Mao, Renduo Liu, Shuo Zhang,* and Jian-Qiang Wang*

13733

dx.doi.org/10.1021/jp5040745

Electrochemical Identification of Molecular Heterogeneity in Binary Redox Self-Assembled Monolayers on Gold

Huihui Tian, Debo Xiang, Huibo Shao,* and Hua-Zhong Yu*

13743

dx.doi.org/10.1021/jp5044255

Studies on SO₂ Tolerance and Regeneration over Perovskite-Type LaCo_{1-x}Pt_xO₃ in NO_x Storage and Reduction

Xiuyun Wang, Xinxin Qi, Zhilin Chen, Lilong Jiang, Ruihu Wang,* and Kemei Wei*

13752

dx.doi.org/10.1021/jp505677f

Electric-Field-Induced Control and Switching of Block Copolymer Domain Orientations in Nanoconfined Channel Architectures

Qianqian Tong and S. J. Sibener*

Plasmonics, Optical Materials, and Hard Matter

13757 

[dx.doi.org/10.1021/jp500831c](https://doi.org/10.1021/jp500831c)

Extraordinary High Microwave Absorption Cross Section of Ultralong Carbon Nanotubes

Jongju Yun, Wonjae Jeon, Lee W. Drahushuk, Seunghyun Baik,* and Michael S. Strano*

13764

[dx.doi.org/10.1021/jp502020g](https://doi.org/10.1021/jp502020g)

Tuning the Aromaticity of *s*-Triazine in the Crystal Phase by Pressure

Samuele Fanetti, Margherita Citroni,* and Roberto Bini

13769

[dx.doi.org/10.1021/jp502084f](https://doi.org/10.1021/jp502084f)

Hydrogenated Grain Boundaries Control the Strength and Ductility of Polycrystalline Graphene

Nan-Nan Li, Zhen-Dong Sha, Qing-Xiang Pei,* and Yong-Wei Zhang*

13775 

[dx.doi.org/10.1021/jp502311z](https://doi.org/10.1021/jp502311z)

Luminescent Properties and Energy Transfer in Pr³⁺ Doped and Pr³⁺-Yb³⁺ Co-doped ZnO Thin Films

M. Balestrieri,* M. Gallart, M. Ziegler, P. Bazylewski, G. Ferblantier, G. Schmerber, G. S. Chang, P. Gilliot, D. Muller, A. Slaoui, S. Colis,* and A. Dinia

13781

[dx.doi.org/10.1021/jp5027493](https://doi.org/10.1021/jp5027493)

Thermal and Optical Characterization of Undoped and Neodymium-Doped Y₃ScAl₄O₁₂ Ceramics

Maria Cinta Pujol,* Alexandre Maitre, Julie Carreau, Rémy Boulesteix, Alain Brenier, Guillaume Alombert-Goget, Yannick Guyot, Joan Josep Carvajal, Rosa Maria Solé, Jaume Massons, Alberto Oleaga, Agustín Salazar, Isabel Gallardo, Pablo Moreno, Javier Rodríguez Vázquez de Aldana, Magdalena Aguiló, and Francesc Diaz

13790

[dx.doi.org/10.1021/jp503106k](https://doi.org/10.1021/jp503106k)

Femtosecond Spectroscopy of Superfluorescent Fluorenyl Benzothiadiazoles with Large Two-Photon and Excited-State Absorption

Kevin D. Belfield,* Mykhailo V. Bondar, Sheng Yao, Ivan A. Mikhailov, Vyacheslav S. Polikanov, and Olga V. Przhonska

13801 

[dx.doi.org/10.1021/jp503505x](https://doi.org/10.1021/jp503505x)

Plasmonic Coupling in Single Silver Nanosphere Assemblies by Polarization-Dependent Dark-Field Scattering Spectroscopy

Xiangdong Tian, Yadong Zhou, Sravan Thota, Shengli Zou, and Jing Zhao*

Physical Processes in Nanomaterials and Nanostructures

13809 

[dx.doi.org/10.1021/jp4098099](https://doi.org/10.1021/jp4098099)

Sliding Properties of MoS₂ Layers: Load and Interlayer Orientation Effects

G. Levita, A. Cavaleiro, E. Molinari, T. Polcar, and M. C. Righi*

13817



dx.doi.org/10.1021/jp501846f

Anaerobic Reaction of Nanoscale Zervalent Iron with Water: Mechanism and Kinetics

Jan Filip, František Karlický, Zdeněk Marušák, Petr Lazar, Miroslav Černík, Michal Otyepka,* and Radek Zbořil*

13826

dx.doi.org/10.1021/jp504429g

Room Temperature Ferromagnetism in Shuttle-like BaMoO₄ Microcrystals

Donglin Guo, Qi Yang, Hao Hua, and Chenguo Hu*

13833



dx.doi.org/10.1021/jp500501e

Defect Enhanced Efficient Physical Functionalization of Graphene with Gold Nanoparticles Probed by Resonance Raman Spectroscopy

Ravi K. Biroju and P. K. Giri*

13844



dx.doi.org/10.1021/jp500578f

Effect of Oleic Acid Concentration on the Physicochemical Properties of Cobalt Ferrite Nanoparticles

Sonja Jovanović, Matjaž Spreitzer,* Melita Tramšek, Zvonko Trontelj, and Danilo Suvorov

13857

dx.doi.org/10.1021/jp500630m

Influence of Nanoscale Confinement on the Molecular Mobility of Ibuprofen

Ana R. Brás, Isabel M. Fonseca, Madalena Dionísio, Andreas Schönhals, Frédéric Affouard, and Natália T. Correia*

13869



dx.doi.org/10.1021/jp500684y

Heterogeneous Gas-Phase Synthesis and Molecular Dynamics Modeling of Janus and Core–Satellite Si–Ag Nanoparticles

Vidyadhar Singh, Cathal Cassidy,* Panagiotis Grammatikopoulos, Flyura Djurabekova, Kai Nordlund, and Mukhles Sowwan

13876



dx.doi.org/10.1021/jp500737c

Examination of Nanoparticle–DNA Binding Characteristics Using Single-Molecule Imaging Atomic Force Microscopy

Kungang Li and Yongsheng Chen*

13883



dx.doi.org/10.1021/jp500872w

Near-Infrared Emitting AgInS₂/ZnS Nanocrystals

Baodong Mao, Chi-Hung Chuang, Christopher McCleese, Junjie Zhu,* and Clemens Burda*

13890

dx.doi.org/10.1021/jp501077t

Reversible Charge-Transfer Doping in Graphene due to Reaction with Polymer Residues

Chenxing Deng, Weiwei Lin,* Guillaume Agnus, Diana Dragoi, Debora Pierucci, Abdelkarim Ouerghi, Sylvain Eimer, Ivanka Barisic, Dafiné Ravelosona, Claude Chappert, and Weisheng Zhao*

13898

[dx.doi.org/10.1021/jp501313r](https://doi.org/10.1021/jp501313r)

Transition Temperature of Wurtzite CoO Nanocrystals as Revealed in Comprehensive Magnetic Characterization

Xuemin He, Wei Zhong,* Shiming Yan, Chao Liu, Huigang Shi, Chak-Tong Au, and Youwei Du

13904



[dx.doi.org/10.1021/jp502038v](https://doi.org/10.1021/jp502038v)

Shape-Dependent Two-Photon Photoluminescence of Single Gold Nanoparticles

Nengyue Gao, Yang Chen, Lin Li, Zhenping Guan, Tingting Zhao, Na Zhou, Peiyan Yuan, Shao Q. Yao, and Qing-Hua Xu*

13912



[dx.doi.org/10.1021/jp502117d](https://doi.org/10.1021/jp502117d)

Micro-Raman Analysis of Three-Dimensional Macroporous Sponge-Like Network of Carbon Nanotubes under Tension

Saveria Santangelo,* Elpida Piperopoulos, Giuliana Faggio, Angela Malara, Enza Fazio, and Candida Milone

13920



[dx.doi.org/10.1021/jp502123n](https://doi.org/10.1021/jp502123n)

Magnitude of the Förster Radius in Colloidal Quantum Dot Solids

A. Jolene Mork, Mark C. Weidman, Ferry Prins, and William A. Tisdale*

13929



[dx.doi.org/10.1021/jp502190y](https://doi.org/10.1021/jp502190y)

NMR Chemical Shifts of ¹⁵N-Bearing Graphene

Xianlong Wang,* Zhufeng Hou, Takashi Ikeda, and Kiyoyuki Terakura

13936



[dx.doi.org/10.1021/jp502267d](https://doi.org/10.1021/jp502267d)

Electromechanical Properties of Carbon Nanotubes

Rosalba Juarez-Mosqueda, Mahdi Ghorbani-Asl, Agnieszka Kuc, and Thomas Heine*

13945



[dx.doi.org/10.1021/jp502790w](https://doi.org/10.1021/jp502790w)

Ultrabright BODIPY-Tagged Polystyrene Nanoparticles: Study of Concentration Effect on Photophysical Properties

Chloé Grazon, Jutta Rieger, Bernadette Charleux, Gilles Clavier,* and Rachel Méallet-Renault*

13953



[dx.doi.org/10.1021/jp5028492](https://doi.org/10.1021/jp5028492)

Metal-Dependent Stability of Pristine and Functionalized Unconventional Dimetallofullerene $M_2@I_h-C_{80}$

Zhiyong Wang, Ryo Kitaura, and Hisanori Shinohara*

13959



[dx.doi.org/10.1021/jp503001s](https://doi.org/10.1021/jp503001s)

Coalescence of Atomically Precise Clusters on Graphenic Surfaces

Atanu Ghosh, Thalappil Pradeep,* and Jaydeb Chakrabarti

13965



[dx.doi.org/10.1021/jp503082g](https://doi.org/10.1021/jp503082g)

SERS Spectra of Oligonucleotides as Fingerprints to Detect Label-Free RNA in Microfluidic Devices

Enora Prado, Annie Colin, Laurent Servant,* and Sophie Lecomte*

13972

[dx.doi.org/10.1021/jp503209y](https://doi.org/10.1021/jp503209y)

Tunable Thermal Transport in Phase Change Materials Using Inverse Micellar Templating and Nanofillers

S. A. Angayarkanni and John Philip*

13981

[dx.doi.org/10.1021/jp503389c](https://doi.org/10.1021/jp503389c)

Magnetic Structure of Ground and Field Induced Ordered States of Low-Dimensional γ - CoV_2O_6

M. Lenertz, A. Dinia, S. Colis,* O. Mentré, G. André, F. Porcher, and E. Suard

13988

[dx.doi.org/10.1021/jp5033977](https://doi.org/10.1021/jp5033977)

Computational Screening of Porous Coordination Networks for Adsorption and Membrane-Based Gas Separations

Tugba Nur Ozturk and Seda Keskin*

13998

[dx.doi.org/10.1021/jp503429k](https://doi.org/10.1021/jp503429k)

Effect of Cation Alkyl Chain Length and Anion Type on Protic Ionic Liquid Nanostructure

Robert Hayes, Silvia Imberti, Gregory G. Warr, and Rob Atkin*

14009

[dx.doi.org/10.1021/jp503442b](https://doi.org/10.1021/jp503442b)

Rapid and Highly Compact Purification for Focused Electron Beam Induced Deposits: A Low Temperature Approach Using Electron Stimulated H_2O Reactions

Barbara Geier, Christian Gspan, Robert Winkler, Roland Schmied, Jason D. Fowlkes, Harald Fitzek, Sebastian Rauch, Johannes Rattenberger, Philip D. Rack, and Harald Plank*

14017

[dx.doi.org/10.1021/jp503503p](https://doi.org/10.1021/jp503503p)

Highly Reactive Pd NCs by Versatile Continuous Supercritical Fluids Synthesis for the Preparation of Metal–Nonmetal Pd-Based NCs

Oana Pascu, Sandy Moisan, Jean-Daniel Marty, and Cyril Aymonier*

14026

[dx.doi.org/10.1021/jp503701k](https://doi.org/10.1021/jp503701k)

Modulation of the Band Gap Increase in Nanocrystals by Surface Passivation

Xin Liu,* Y. Y. Sun,* D. West, Xingfa Gao, and S. B. Zhang*

14031

[dx.doi.org/10.1021/jp503828x](https://doi.org/10.1021/jp503828x)

Spatially Selective Au Nanoparticle Deposition and Raman Analysis of Ion-Irradiated Single-Wall Carbon Nanotubes

Nathanael D. Cox, Jamie E. Rossi, Cory D. Cress, Andrew Merrill, Kyle R. Crompton, and Brian J. Landi*

14039

[dx.doi.org/10.1021/jp504083g](https://doi.org/10.1021/jp504083g)

Resolving and Quantifying Nanoscaled Phases in Amorphous FeF_3 by Pair Distribution Function and Mössbauer Spectroscopy

Damien Dambournet,* Mathieu Duttine, Karena W. Chapman, Alain Wattiaux, Olaf Borkiewicz, Peter J. Chupas, Alain Demourgues, and Henri Grout

14044

[dx.doi.org/10.1021/jp5042603](https://doi.org/10.1021/jp5042603)

Formation of Ordered vs Disordered Carbon Nanotube Serpentines on Anisotropic vs Isotropic Substrates

Nitzan Shadmi, Noam Geblinger, Ariel Ismach, and Ernesto Joselevich*

14051



[dx.doi.org/10.1021/jp505257g](https://doi.org/10.1021/jp505257g)

Phosphorene Nanoribbons, Phosphorus Nanotubes, and van der Waals Multilayers

Hongyan Guo, Ning Lu, Jun Dai, Xiaojun Wu,* and Xiao Cheng Zeng*

Additions and Corrections

14060

[dx.doi.org/10.1021/jp504161c](https://doi.org/10.1021/jp504161c)

Correction to "Effect of Different Surfactants on the Size Control and Optical Properties of $\text{Y}_2\text{O}_3:\text{Eu}^{3+}$ Nanoparticles Prepared by Coprecipitation Method"

Abhijit P. Jadhav, Chang Woo Kim, Hyun Gil Cha, Amol Uttam Pawar, Nitin Appa Jadhav, U. Pal, and Young Soo Kang*