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J80/pc2

MAY 1, 2014

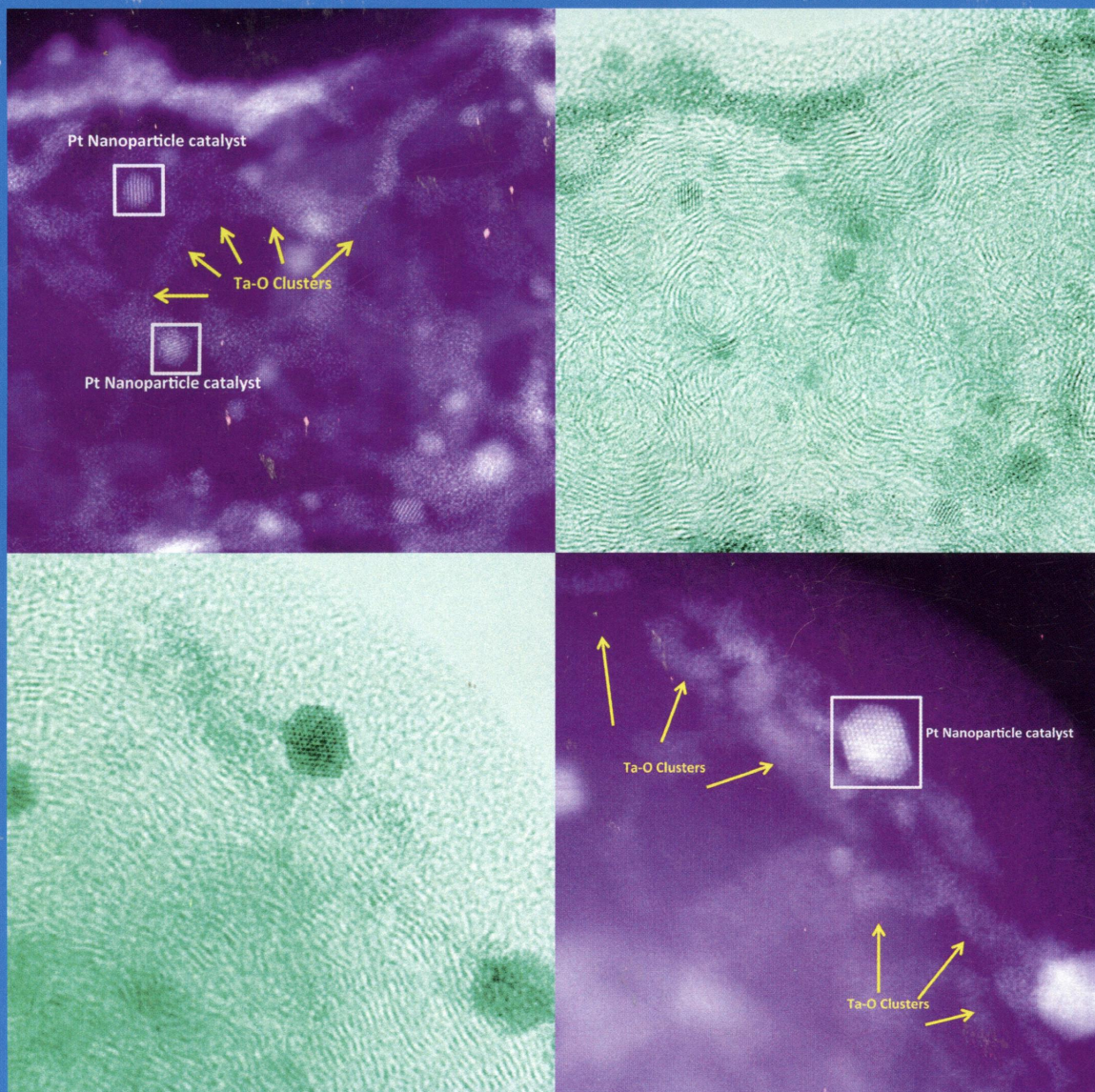
VOLUME 118

NUMBER 17

pubs.acs.org/JPCC

# THE JOURNAL OF PHYSICAL CHEMISTRY

# C



**Strong Metal-Support  
Interaction (SMSI):  
Pt Nanocatalysts  
Surrounded by  
Clusters of Tantalum  
Oxide over a  
Carbon Support  
(see page 8723)**

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



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**ON THE COVER:** Strong metal-support interaction (SMSI): Pt nanocatalysts surrounded by clusters of tantalum oxide over a carbon support. Atomic-resolution scanning transmission electron microscopy (STEM) images demonstrating a Pt catalyst strongly interacting with a hybrid support of Ta-O clusters over carbon. Top right: high-angle annular dark-field (HAADF) STEM micrograph of the Pt catalysts over the support demonstrating the heavy atoms from the Pt nanoparticles and Ta network. Top left: corresponding high-resolution bright-field STEM image of the same region (acquired simultaneously as the HAADF STEM image) clearly showing the graphitic fringes of the carbon support. Full size of the field of view is approximately 40 nm x 40 nm. Bottom right: detailed high-resolution bright-field STEM image of a different region of the same catalyst. Bottom left: corresponding HAADF STEM micrograph of the same region showing highlights of the complex hybrid structure of the graphitic carbon, the oxide, and Pt nanocatalysts. Full size of the field of view is 27 nm x 27 nm. Images are colorized with a uniform palette for artistic purposes only. See page 8723.

## Feature Article

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[dx.doi.org/10.1021/jp412292w](https://doi.org/10.1021/jp412292w)

**Primary Oxide Latent Storage and Spillover Enabling Electrocatalysts with Reversible Oxygen Electrode Properties and the Alterpolar Reversible (PEMFC versus WE) Cell**

Milan M. Jaksic, Gianluigi A. Botton, Georgios D. Papakonstantinou, Feihong Nan, and Jelena M. Jaksic\*

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[dx.doi.org/10.1021/jp409733a](https://doi.org/10.1021/jp409733a)

**Optical Enhancement in Heteroleptic Ru(II) Polypyridyl Complexes Using Electron-Donor Ancillary Ligands**

Rui Dong, Arrigo Calzolari, Rosa di Felice, Ahmed El-Shafei, Maqbool Hussain, and Marco Buongiorno Nardelli\*

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[dx.doi.org/10.1021/jp4124265](https://doi.org/10.1021/jp4124265)

**Multiple-Anchoring Triphenylamine Dyes for Dye-Sensitized Solar Cell Application**

Guohua Wu, Fantai Kong,\* Yaohong Zhang, Xianxi Zhang,\* Jingzhe Li, Wangchao Chen, Weiqing Liu, Yong Ding, Changneng Zhang, Bing Zhang, Jianxi Yao, and Songyuan Dai\*

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**Theory for Anomalous Electric Double-Layer Dynamics in Ionic Liquids**

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**Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles**

Guido Fratesi,\* Carlo Motta, Mario Italo Trioni, Gian Paolo Brivio, and Daniel Sánchez-Portal

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[dx.doi.org/10.1021/jp5005743](https://doi.org/10.1021/jp5005743)**Energy Harvesting from the Mixture of Water and Ethanol Flowing through Three-Dimensional Graphene Foam**

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[dx.doi.org/10.1021/jp500796e](https://doi.org/10.1021/jp500796e)**Adsorption and Diffusion of CO<sub>2</sub> and CH<sub>4</sub> in Zeolitic Imidazolate Framework-8: Effect of Structural Flexibility**

Liling Zhang,\* Gang Wu, and Jianwen Jiang\*

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[dx.doi.org/10.1021/jp500870v](https://doi.org/10.1021/jp500870v)**Rapid Electron Injection in Nitrogen- and Fluorine-Doped Flower-Like Anatase TiO<sub>2</sub> with {001} Dominated Facets and Dye-Sensitized Solar Cells with a 52% Increase in Photocurrent**

Jia Yu, Yulin Yang,\* Ruiqing Fan,\* Liang Li, and Xinyuan Li

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[dx.doi.org/10.1021/jp501140r](https://doi.org/10.1021/jp501140r)**Photophysical Characterization of a Ruthenium(II) Tris(2,2'-bipyridine)-Doped Zirconium UiO-67 Metal–Organic Framework**

William A. Maza and Amanda J. Morris\*

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[dx.doi.org/10.1021/jp5016966](https://doi.org/10.1021/jp5016966)**FeO<sub>x</sub>-Coated SnO<sub>2</sub> as an Anode Material for Lithium Ion Batteries**

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[dx.doi.org/10.1021/jp501819p](https://doi.org/10.1021/jp501819p)**Hydrogenation Synthesis of Blue TiO<sub>2</sub> for High-Performance Lithium-Ion Batteries**

Jingxia Qiu, Sheng Li, Evan Gray, Hongwei Liu, Qin-Fen Gu, Chenghua Sun, Chao Lai, Huijun Zhao, and Shanqing Zhang\*

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[dx.doi.org/10.1021/jp502057p](https://doi.org/10.1021/jp502057p)**Growth of 2D ZnO Nanowall for Energy Harvesting Application**

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[dx.doi.org/10.1021/jp502948y](https://doi.org/10.1021/jp502948y)**Understanding the Apparent Charge Density Dependence of Mobility and Lifetime in Organic Bulk Heterojunction Solar Cells**

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[dx.doi.org/10.1021/jp4098205](https://doi.org/10.1021/jp4098205)**Characterization of the Dehydrogenation Process of LiBH<sub>4</sub> Confined in Nanoporous Carbon**

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Tim Mason and E. H. Majzoub\*

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**Determination of the Apparent Crystal Structure of a Highly Faulted UPRM-5 Type Flexible Porous Titanium Silicate via a Polymorph Based Superposition Model, a Rietveld Refinement and a Pair Distribution Function**

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[dx.doi.org/10.1021/jp4087943](https://doi.org/10.1021/jp4087943)

**Theoretical Study of the Deposition of Pt Clusters on Defective Hexagonal Boron Nitride (*h*-BN) Sheets: Morphologies, Electronic Structures, and Interactions with O**

Duo Xu, Yue-jie Liu, Jing-xiang Zhao,\* Qing-hai Cai, and Xuan-zhang Wang\*

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**Comparative Study of Homogeneous and Heterogeneous Photocatalytic Degradation of RhB under Visible Light Irradiation with Keggin-Type Manganese-Substituted Catalysts**

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**Toward Efficient Drug Delivery through Suitably Prepared Metal–Organic Frameworks: A First-Principles Study**

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**Cu(II) as a General Cocatalyst for Improved Visible-Light Photocatalytic Performance of Photosensitive Ag-Based Compounds**

Ping Wang, Yang Xia, Panpan Wu, Xuefei Wang, Huogen Yu,\* and Jianguo Yu

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[dx.doi.org/10.1021/jp410716q](https://doi.org/10.1021/jp410716q)

**Spin Switch of the Transition-Metal-Doped Boron Nitride Sheet through H/F Chemical Decoration**

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**Immobilizing Metal Nanoparticles on Single Wall Nanotubes. Effect of Surface Curvature**

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[dx.doi.org/10.1021/jp410794j](https://doi.org/10.1021/jp410794j)**Photocatalytic Current Doubling-Induced Generation of Uniform Selenium and Cadmium Selenide Quantum Dots on Titanium(IV) Oxide**

Musashi Fujishima, Kentaro Tanaka, Naoki Sakami, Masataka Wada, Katsuyuki Morii, Takanori Hattori, Yasutaka Sumida, and Hiroaki Tada\*

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[dx.doi.org/10.1021/jp4116707](https://doi.org/10.1021/jp4116707)**Influence of Organic Amino and Thiol Ligands on the Geometric and Electronic Surface Properties of Colloidally Prepared Platinum Nanoparticles**

Lena Altmann, Sebastian Kunz,\* and Marcus Bäumer

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[dx.doi.org/10.1021/jp412160e](https://doi.org/10.1021/jp412160e)**Elastic Properties of Swelling Clay Particles at Finite Temperature upon Hydration**

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[dx.doi.org/10.1021/jp4123002](https://doi.org/10.1021/jp4123002)**Alumina(0001)/Water Interface: Structural Properties and Infrared Spectra from First-Principles Molecular Dynamics Simulations**

Patrick Huang,\* Tuan Anh Pham, Giulia Galli, and Eric Schwegler

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[dx.doi.org/10.1021/jp412505p](https://doi.org/10.1021/jp412505p)**Localized Impedance Measurements for Electrochemical Surface Science**

Aliaksandr S. Bandarenka,\* Artjom Maljusch, Volodymyr Kuznetsov, Kathrin Eckhard, and Wolfgang Schuhmann\*

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[dx.doi.org/10.1021/jp412539y](https://doi.org/10.1021/jp412539y)**Atomic Layer Deposition of Platinum Nanoparticles on Titanium Oxide and Tungsten Oxide Using Platinum(II) Hexafluoroacetylacetonate and Formalin as the Reactants**

Virginia R. Anderson, Noemi Leick, Joel W. Clancey, Katherine E. Hurst, Kim M. Jones, Anne C. Dillon, and Steven M. George\*

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[dx.doi.org/10.1021/jp412756a](https://doi.org/10.1021/jp412756a)**Periodic DFT+D Molecular Modeling of the Zn-MOF-5(100)/(110)TiO<sub>2</sub> Interface: Electronic Structure, Chemical Bonding, Adhesion, and Strain**

Filip Zasada,\* Witold Piskorz, Joanna Gryboś, and Zbigniew Sojka

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[dx.doi.org/10.1021/jp500041v](https://doi.org/10.1021/jp500041v)**Carbon Coated Silica Doped With Cerium/Zirconium Mixed Oxides as NO<sub>2</sub> Adsorbent at Ambient Conditions**

Amani M. Ebrahim and Teresa J. Bandosz\*

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[dx.doi.org/10.1021/jp500751a](https://doi.org/10.1021/jp500751a)**Few-Layer Graphene-Encapsulated Metal Nanoparticles for Surface-Enhanced Raman Spectroscopy**

Youming Liu, Yue Hu, and Jin Zhang\*

8999  [dx.doi.org/10.1021/jp500781v](https://doi.org/10.1021/jp500781v)

**Elucidating Oxygen Reduction Active Sites in Pyrolyzed Metal–Nitrogen Coordinated Non-Precious-Metal Electrocatalyst Systems**

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9009  [dx.doi.org/10.1021/jp500797x](https://doi.org/10.1021/jp500797x)

**Self-Assembly of a Monolayer Graphene Oxide Film Based on Surface Modification of Substrates and its Vapor-Phase Reduction**

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9018 [dx.doi.org/10.1021/jp500806w](https://doi.org/10.1021/jp500806w)

**Making C–C Bonds with Gold Catalysts: A Theoretical Study of the Influence of Gold Particle Size on the Dissociation of the C–X Bond in Aryl Halides**

Mercedes Boronat,\* Tirso López-Ausens, and Avelino Corma

9030  [dx.doi.org/10.1021/jp5009384](https://doi.org/10.1021/jp5009384)

**Improving the CO-PROX Performance of Inverse CeO<sub>2</sub>/CuO Catalysts: Doping of the CuO Component with Zn**

A. López Cámara,\* V. Cortés Corberán, L. Barrio, G. Zhou, R. Si, J. C. Hanson, M. Monte, J. C. Conesa, J. A. Rodríguez,\* and A. Martínez-Arias\*

9042 [dx.doi.org/10.1021/jp501201b](https://doi.org/10.1021/jp501201b)

**CO<sub>2</sub> Adsorption As a Flat-Lying, Tridentate Carbonate on CeO<sub>2</sub>(100)**

Peter M. Albrecht, De-en Jiang, and David R. Mullins\*

9051  [dx.doi.org/10.1021/jp501338k](https://doi.org/10.1021/jp501338k)


**Two-Dimensional Self-Assembled Gold Silicide Honeycomb Nanonetwork on Si(111)7×7**

Fatemeh R. Rahsepar, Lei Zhang, and K. T. Leung\*

9056  [dx.doi.org/10.1021/jp5014847](https://doi.org/10.1021/jp5014847)

**Effect of the Confinement and Presence of Cations on Hydrogen Bonding of Water in LTA-Type Zeolite**

S. Calero and P. Gómez-Álvarez\*

9066  [dx.doi.org/10.1021/jp501608b](https://doi.org/10.1021/jp501608b)


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9073 [dx.doi.org/10.1021/jp501825e](https://doi.org/10.1021/jp501825e)

**Passivation of Nickel Nanoneedles in Aqueous Solutions**

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9078  [dx.doi.org/10.1021/jp501940f](https://doi.org/10.1021/jp501940f)  
**An Efficient Cu/BaO/La<sub>2</sub>O<sub>3</sub> Catalyst for the Simultaneous Removal of Carbon Soot and Nitrogen Oxides from Simulated Diesel Exhaust**  
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9086 [dx.doi.org/10.1021/jp502137j](https://doi.org/10.1021/jp502137j)  
**Computational Study of Propylene and Propane Binding in Metal–Organic Frameworks Containing Highly Exposed Cu<sup>+</sup> or Ag<sup>+</sup> Cations**  
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9093  [dx.doi.org/10.1021/jp502949q](https://doi.org/10.1021/jp502949q)  
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**Effects of Organic Moieties on Luminescence Properties of Organic–Inorganic Layered Perovskite-Type Compounds**  
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9114  [dx.doi.org/10.1021/jp412821w](https://doi.org/10.1021/jp412821w)  
**Two-Dimensional Array of Silica Particles as a SERS Substrate**  
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**Direct Near-Field Observation of Orientation-Dependent Optical Response of Gold Nanorods**  
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**Variable Range Hopping Conduction in BaTiO<sub>3</sub> Ceramics Exhibiting Colossal Permittivity**  
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[dx.doi.org/10.1021/jp5023423](https://doi.org/10.1021/jp5023423) **$^{127}\text{I}$  and  $^{207}\text{Pb}$  Solid-State NMR Spectroscopy and Nuclear Spin Relaxation in  $\text{PbI}_2$ : A Preliminary Study**

R. E. Taylor, Peter A. Beckmann, Shi Bai, and C. Dybowski\*

**Physical Processes in Nanomaterials and Nanostructures**

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[dx.doi.org/10.1021/jp411011c](https://doi.org/10.1021/jp411011c)**Local Structure Investigation of Cobalt and Manganese Doped ZnO Nanocrystals and Its Correlation with Magnetic Properties**

S. Basu, D. Y. Inamdar, Shailaja Mahamuni, Apama Chakrabarti, C. Kamal, G. Ravi Kumar, S. N. Jha, and D. Bhattacharyya\*

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[dx.doi.org/10.1021/jp4110932](https://doi.org/10.1021/jp4110932)**Complex Impedance Spectroscopy Study of the Thermolysis Products of Metal–Organic Frameworks**

Serguei D. Mikhailenko, Foroughazam Afsahi, and Serge Kaliaguine\*

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[dx.doi.org/10.1021/jp411953d](https://doi.org/10.1021/jp411953d)**Structure Analysis of Al-Modified  $\text{TiO}_2$  Nanocatalyst Supports**

Rebecca E. Olsen, Todd M. Alam, Calvin H. Bartholomew, David B. Enfield, and Brian F. Woodfield\*

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[dx.doi.org/10.1021/jp412320w](https://doi.org/10.1021/jp412320w)**CO Adsorption on Ag Nanoclusters Supported on Carbon Nanotube: A Molecular Dynamics Study**

Hamed Akbarzadeh,\* Hamzeh Yaghoubi, Amir Nasser Shamkhali, and Farid Taherkhani

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[dx.doi.org/10.1021/jp500024h](https://doi.org/10.1021/jp500024h)**Porphyrin–Nanoclay Photosensitizers for Visible Light Induced Oxidation of Phenol in Aqueous Media**

Dominik Drozd, Krzysztof Szczubialka, Michał Skiba, Mariusz Kepczynski, and Maria Nowakowska\*

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[dx.doi.org/10.1021/jp500050r](https://doi.org/10.1021/jp500050r)**Vapor Phase Growth and Imaging Stacking Order of Bilayer Molybdenum Disulfide**

Shengxue Yang,\* Jun Kang, Qu Yue, and Kun Yao

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[dx.doi.org/10.1021/jp500516t](https://doi.org/10.1021/jp500516t)**Core–Shell  $\text{In}_2\text{O}_3/\text{ZnO}$  Nanopillar Nanogenerator as a Self-Powered Active Gas Sensor with High  $\text{H}_2\text{S}$  Sensitivity and Selectivity at Room Temperature**

Weili Zang, Yuxin Nie, Dan Zhu, Ping Deng, Lili Xing,\* and Xinyu Xue\*

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[dx.doi.org/10.1021/jp5007395](https://doi.org/10.1021/jp5007395)**Mechanism of Nonlinear Optical Enhancement and Supramolecular Isomerism in 1D Polymeric Zn(II) and Cd(II) Sulfates with Pyridine-4-aldoxime Ligands**

Lilia Croitor, Eduard B. Coropceanu, Artëm E. Masunov,\* Hector J. Rivera-Jacquez, Anatolii V. Siminel, and Marina S. Fonari\*



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[dx.doi.org/10.1021/jp5010083](https://doi.org/10.1021/jp5010083)

**Comments on the Energy Barrier Calculations during “Stick–Slip” Behavior of Evaporating Droplets Containing Nanoparticles**

Melik Oksuz and H. Yildirim Erbil\*

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[dx.doi.org/10.1021/jp501039w](https://doi.org/10.1021/jp501039w)

**Probing the Quenching of Quantum Dot Photoluminescence by Peptide-Labeled Ruthenium(II) Complexes**

Amy M. Scott,\* W. Russ Algar, Michael H. Stewart, Scott A. Trammell, Juan B. Blanco-Canosa, Philip E. Dawson, Jeffrey R. Deschamps, Ramasis Goswami, Eunkeu Oh, Alan L. Huston, and Igor L. Medintz\*

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[dx.doi.org/10.1021/jp5013158](https://doi.org/10.1021/jp5013158)

**Versatile Electronic and Magnetic Properties of SnSe<sub>2</sub> Nanostructures Induced by the Strain**

Yucheng Huang,\* Chongyi Ling, Hai Liu, Sufan Wang, and Baoyou Geng\*

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[dx.doi.org/10.1021/jp501345f](https://doi.org/10.1021/jp501345f)

**Pluronic-Silica (PluS) Nanoparticles Doped with Multiple Dyes Featuring Complete Energy Transfer**

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[dx.doi.org/10.1021/jp501792j](https://doi.org/10.1021/jp501792j)

**Phase Behavior of DNA-Stabilized Carbon Nanotubes Dispersions: Association with Oppositely-Charged Additives**

Franco Tardani\* and Simona Sennato

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[dx.doi.org/10.1021/jp5018345](https://doi.org/10.1021/jp5018345)

**Microsecond Transient Absorption Spectra of Suspended Semiconducting Metal Oxide Nanoparticles**

Herme G. Baldovi, Belén Ferrer, Mercedes Álvaro, and Hermenegildo García\*

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[dx.doi.org/10.1021/jp5019636](https://doi.org/10.1021/jp5019636)

**Förster-Induced Energy Transfer in Functionalized Graphene**

Ermin Malic,\* Heiko Appel, Oliver T. Hofmann, and Angel Rubio\*

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[dx.doi.org/10.1021/jp502174b](https://doi.org/10.1021/jp502174b)

**Understanding How in Situ Generated Hydrogen Controls the Morphology of Platinum Nanoparticles**

Neus Aguilera-Porta, Monica Calatayud,\* Caroline Salzemann, and Christophe Petit\*

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[dx.doi.org/10.1021/jp5029678](https://doi.org/10.1021/jp5029678)

**Hexagonalization of Aluminogermanate Imogolite Nanotubes Organized into Closed-Packed Bundles**

Mohamed Salah Amara, Stéphan Rouzière, Erwan Paineau, Maria Bacía-Verloop, Antoine Thill,\* and Pascale Launois\*

## Additions and Corrections

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[dx.doi.org/10.1021/jp503563s](https://doi.org/10.1021/jp503563s)

**Correction to “Optical Tracking of Single Ag Clusters in Nanostructured Water Films”**

Stefan Krause,\* Martin Hartmann, Ingolf Kahle, Martin Neumann, Mario Heidernätsch, Stefan Spange, and Christian von Borczyskowski