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J80/po2

DECEMBER 11, 2014

VOLUME 118

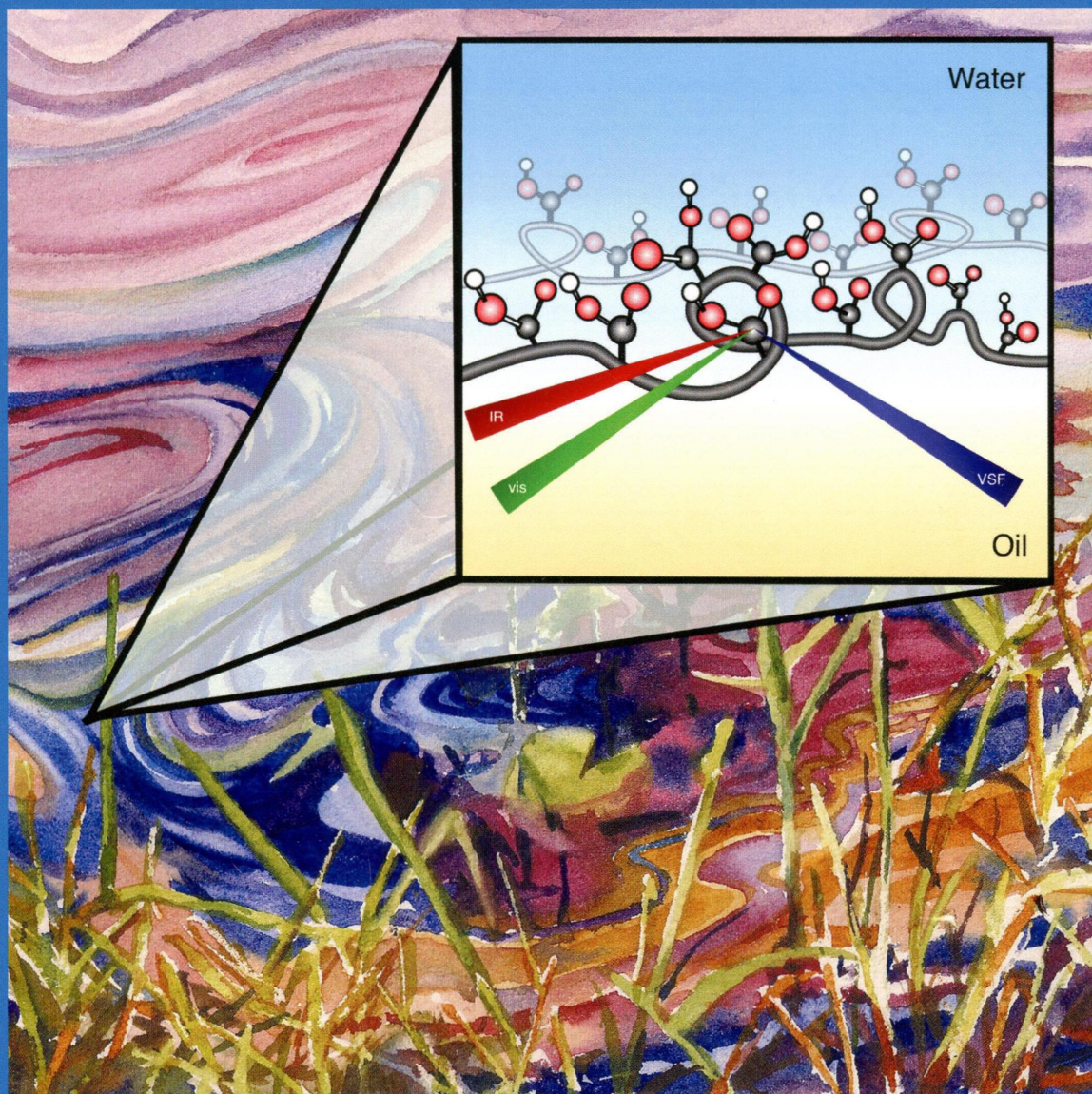
NUMBER 49

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THE JOURNAL OF PHYSICAL CHEMISTRY

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From Order to Disorder:
Multilayer Assembly of
Polyelectrolytes at an
Oil–Water Interface
(see page 28331)



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



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ON THE COVER: From order to disorder: multilayer assembly of polyelectrolytes at an oil–water interface. Knowing the conditions under which polyelectrolytes adsorb to and assemble at an oil–water interface is important to many fields ranging from water remediation to enhanced oil recovery. Vibrational sum-frequency spectroscopic studies have revealed that this assembly process for carboxylic-acid-containing polyelectrolytes occurs through a unique multistep process that depends on a variety of factors, including the degree of polyelectrolyte charging, the configuration of the polyelectrolyte backbone, and the binding of salt cations to the charged carboxylate groups. Watercolor background by Mary M. Robertson. See page 28331.

Feature Article

28331

DOI: 10.1021/jp5068022

Molecular Insights in the Structure and Layered Assembly of Polyelectrolytes at the Oil/Water Interface

Ellen J. Robertson and Geraldine L. Richmond*

Articles

Energy Conversion and Storage; Energy and Charge Transport

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DOI: 10.1021/jp5050145

Modeling of Lead Halide Perovskites for Photovoltaic Applications

Radi A. Jishi,* Oliver B. Ta, and Adel A. Sharif

28350

DOI: 10.1021/jp505386u

Insight into the Li Ion Dynamics in $\text{Li}_{12}\text{Si}_7$: Combining Field Gradient Nuclear Magnetic Resonance, One- and Two-Dimensional Magic-Angle Spinning Nuclear Magnetic Resonance, and Nuclear Magnetic Resonance Relaxometry

Alexander Kuhn, Sven Dupke, Miriam Kunze, Sreeraj Puravankara, Thorsten Langer, Rainer Pöttgen, Martin Winter, Hans-Dieter Wiemhöfer, Hellmut Eckert,* and Paul Heitjans*

28361



DOI: 10.1021/jp5071506

Mechanisms of Magnesium Ion Transport in Pyrrolidinium Bis(trifluoromethanesulfonyl)imide-Based Ionic Liquid Electrolytes

Sebastian Jeremias, Guinevere A. Giffin,* Arianna Moretti, Sangsik Jeong, and Stefano Passerini*

28369



DOI: 10.1021/jp507723n

New Desolvated Gel Electrolyte for Rechargeable Lithium Metal Sulfurized Polyacrylonitrile (S-PAN) Battery

Borong Wu, Qi Liu, Daobin Mu,* Yonghuan Ren, Yu Li, Lei Wang, Hongliang Xu, and Feng Wu

28377 **S**

DOI: 10.1021/jp507952b

Composition as a Means To Control Morphology and Properties of Epoxy Based Dual-Phase Structural Electrolytes
Natasha Shirshova,* Alexander Bismarck, Emile S. Greenhalgh, Patrik Johansson,* Gerhard Kalinka, Maciej J. Marczewski,
Milo S. P. Shaffer, and Malte Wienrich

28388 **S**

DOI: 10.1021/jp507984s

Design of Efficient Photoinduced Charge Separation in Donor–Copper(I)–Acceptor Triad
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and Fabrice Odobel*

28401 **S**

DOI: 10.1021/jp5080847

Reduced Graphene Oxide Paper Electrode: Opposing Effect of Thermal Annealing on Li and Na Cyclability
Lamuel David and Gurpreet Singh*

28409

DOI: 10.1021/jp508780b

Effect of the Partial Replacement of CaH₂ with CaF₂ in the Mixed System CaH₂ + MgB₂
C. Pistidda,* F. Karimi, S. Garroni, A. Rzeszutek, C. Bonatto Minella, C. Milanese, T. T. Le, L. H. Rude, J. Skibsted, T. R. Jensen,
C. Horstmann, C. Gundlach, M. Tolkiehn, P. K. Pranzas, A. Schreyer, T. Klassen, and M. Dornheim

28418 **S**

DOI: 10.1021/jp508799j

Carrier Dynamics in Pentacene/C₆₀ Bilayer Solar Cell Investigated through the Magnetoconductance
Takuya Omori, Yusuke Wakikawa, Tomoaki Miura, Yuji Yamaguchi, Ken-ichi Nakayama, and Tadaaki Ikoma*

28425 **S**

DOI: 10.1021/jp5088338

Dye-Anchoring Functional Groups on the Performance of Dye-Sensitized Solar Cells: Comparison between Alkoxysilyl and Carboxyl Groups
Sri Kasi Matta, Kenji Kakiage, Satoshi Makuta, Aisea Veamatahau, Yohei Aoyama, Toru Yano, Minoru Hanaya,* and
Yasuhiro Tachibana*

28435 **S**

DOI: 10.1021/jp5088465

Transition Metal Complexes with Macrocyclic Ligands Serve as Efficient Electrocatalysts for Aprotic Oxygen Evolution on Li₂O₂
Shoichi Matsuda, Shigeki Mori, Kazuhito Hashimoto,* and Shuji Nakanishi*

28440


DOI: 10.1021/jp509182g


Enhanced Electrochemical Performance of Reduced Graphene Oxides by H₂/Ar Plasma Treatment
Jie Li, Changlun Chen,* Juan Wei, Jiaying Li, and Xiangke Wang*


28448 **S**

DOI: 10.1021/jp509193h


Ion Transport in Electrolytes for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study
José Manuel Vicent-Luna, Jesús Idígoras, Said Hamad, Sofia Calero, and Juan Antonio Anta*


28456  DOI: 10.1021/jp509223d
Intermediate Phases during Decomposition of Metal Borohydrides, $M(\text{BH}_4)_n$ ($M = \text{Na}, \text{Mg}, \text{Y}$)
Yuzhen Liu, Santanab Giri, Jian Zhou, and Purusottam Jena*


28462  DOI: 10.1021/jp509369n
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Changwen Liu, Zeliang Qiu, Wenjin Yue, Xun Zhou, and Mingtai Wang*

28474  DOI: 10.1021/jp509439g
Compact Self-Assembled Porphyrin Macrocycle: Synthesis, Cooperative Enhancement, and Ultrafast Response
Oleg Varnavski, Jeffery E. Raymond, Zin Seok Yoon, Takefumi Yotsutuji, Kazuya Ogawa,* Yoshiaki Kobuke,* and Theodore Goodson III*


28482 DOI: 10.1021/jp509650v
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28494  DOI: 10.1021/jp509753p
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Ashok Bera, Kewei Wu, Arif Sheikh, Erkki Alarousu, Omar F. Mohammed,* and Tom Wu*

28502  DOI: 10.1021/jp509783h
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Yan Xu, Xiaoshu Zhu, Xiaosi Zhou,* Xia Liu, Yunxia Liu, Zhihui Dai,* and Jianchun Bao

28509  DOI: 10.1021/jp509971q
Excited State and Injection Dynamics of Triphenylamine Sensitizers Containing a Benzothiazole Electron-Accepting Group on TiO_2 and Al_2O_3 Thin Films
Mihalis Fakis,* Peter Hrobárik,* Oleksandr Yushchenko, Ivica Sigmundová, Marius Koch, Arnulf Rosspeintner, Elias Stathatos, and Eric Vauthey*

28520 DOI: 10.1021/jp510147z
Probing Ion Exchange in the Triflic Acid–Guanidinium Triflate System: A Solid-State Nuclear Magnetic Resonance Study
Haijin Zhu,* Douglas MacFarlane, and Maria Forsyth


28527  DOI: 10.1021/jp510701w
Hot Excitons Increase the Donor/Acceptor Charge Transfer Yield
Michael Schulze,* Marc Hänsel, and Petra Tegeder*

28535  DOI: 10.1021/jp5113558
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John M. Papanikolas,* and Kirk S. Schanze*


28542  DOI: 10.1021/jp511362s
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Shuai Liang,* Lizhi Yi, and Deqing Liang

Surfaces, Interfaces, Porous Materials, and Catalysis

28548 DOI: 10.1021/jp501880r
Sensing Mechanism of SnO₂ (110) Surface to CO: Density Functional Theory Calculations
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28562  DOI: 10.1021/jp505663c
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28572 DOI: 10.1021/jp507458q
Basicity of Stereoregulating Electron-Donor Compounds in Ziegler–Natta Catalysts: A Study by Infrared Spectroscopy and Chemical Exchange Reactions
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Michael Severance and Prabir K. Dutta*

28592 DOI: 10.1021/jp5078104
Molecular Exchange in a Heteromolecular PTCDA/CuPc Bilayer Film on Ag(111)
Benjamin Stadtmüller,* Marco Gruenewald, Julia Peuker, Roman Forker, Torsten Fritz, and Christian Kumpf

28603  DOI: 10.1021/jp508382v
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Brice Russell, Jhonny Villaroel, Karim Sapag, and Aldo D. Migone*


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First-Principles Prediction of Oxygen Reduction Activity on Pd–Cu–Si Metallic Glasses
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28616  DOI: 10.1021/jp5089349
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Zhaoyong Guan, Weiyi Wang, Jing Huang,* Xiaojun Wu, Qunxiang Li,* and Jinlong Yang


28625  DOI: 10.1021/jp509041b
Competitive Influence of Hydrogen Bonding and van der Waals Interactions on Self-Assembled Monolayers of Stilbene-Based Carboxylic Acid Derivatives
Ling-yan Liao, Yi-bao Li, Jing Xu, Yan-fang Geng,* Jun-yong Zhang, Jing-li Xie,* Qing-dao Zeng,* and Chen Wang*


28631 DOI: 10.1021/jp509272k
Interfacial Fresnel Coefficients and Molecular Structures of Model Cell Membranes: From a Lipid Monolayer to a Lipid Bilayer
Bolin Li, Xiaolin Lu,* Xiaofeng Han, Fu-Gen Wu, John N. Myers, and Zhan Chen*

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Comparative Electrochemical Investigations in Ionic Liquids and Molecular Solvents of a Carbon Surface Modified by a Redox Monolayer
Joanna Jalkh, Yann R. Leroux, Corinne Lagrost, and Philippe Hapiot*

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28679  DOI: 10.1021/jp509574s
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Emilia A. Carbonio,* Mauricio J. Prieto,* Abner de Siervo, and Richard Landers

28689  DOI: 10.1021/jp5096213
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Zheng Zhang and Ignacio Melián-Cabrera*

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M. Errahali, G. Gatti, L. Tei, G. Paul, G. A. Rolla, L. Canti, A. Fraccarollo, M. Cossi, A. Comotti, P. Sozzani, and L. Marchese*

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DOI: 10.1021/jp509890z

Coarse-Graining of Adsorption in Microporous Materials: Relation between Occupancy Distributions and Local Partition Functions

Federico G. Pazzona,* Pierfranco Demontis, and Giuseppe B. Suffritti

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DOI: 10.1021/jp509970y

Collective Diffusion of Gold Clusters and F-Centers at MgO(100) and CaO(100) Surfaces

Željko Šljivančanin*

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DOI: 10.1021/jp510069q

Structural Transformations of Zinc Oxide Layers on Pt(111)

Bo-Hong Liu, Martin E. McBriarty, Michael J. Bedzyk, Shamil Shaikhutdinov,* and Hans-Joachim Freund

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DOI: 10.1021/jp510114j

Submicrometric Picture of Plaster Hydration: Dynamic and Space-Resolved Raman Spectroscopy versus Kinetic Monte Carlo Simulations

Suzanne Joiret, Françoise Pillier, and Annie Lemarchand*

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DOI: 10.1021/jp510176h

Property of Pt–Ag Alloy Nanoparticle Catalysts in Carbon Monoxide Oxidation

Sang Youp Hwang, Changlin Zhang, Eric Yurchekfrod, and Zhenmeng Peng*

Plasmonics, Optical Materials, and Hard Matter

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DOI: 10.1021/jp506681k

Large Nonlinear Optical Responses of Dimers Bearing a Donor and Acceptor: Long, Intradimer Multicenter Bonding

Wen-Yong Wang, Yu-He Kan,* Li Wang, Shi-Ling Sun, and Yong-Qing Qiu*

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DOI: 10.1021/jp507036h

Highly Efficient Bipolar Host Materials with Indenocarbazole and Pyrimidine Moieties for Phosphorescent Green Light-Emitting Diodes

Gyeong Heon Kim, Raju Lampande, Mi Jin Park, Hyeong Woo Bae, Ji Hoon Kong, Jang Hyuk Kwon,* Jung Hwan Park,* Yong Wook Park, and Choong Eui Song

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DOI: 10.1021/jp5073457

Nonlinear Absorbing Cationic Bipyridyl Iridium(III) Complexes Bearing Cyclometalating Ligands with Different Degrees of π -Conjugation: Synthesis, Photophysics, and Reverse Saturable Absorption

Zhongjing Li, Peng Cui, Chengzhe Wang, Svetlana Kilina, and Wenfang Sun*

28776  DOI: 10.1021/jp507957n

Effects of Concentration, Crystal Structure, Magnetism, and Electronic Structure Method on First-Principles Oxygen Vacancy Formation Energy Trends in Perovskites

Matthew T. Cuman and John R. Kitchin*

28791 DOI: 10.1021/jp5092587

Metal-Enhanced S₁ and Alpha- S₂ Fluorescence: Effects of Far-Field Excitation Irradiance on Enhanced Fluorescence

Hirdyesh Mishra and Chris D. Geddes*

28797 DOI: 10.1021/jp5095883

Atomic Displacive Disorder in Bi₂Ti₂O₇

Christopher Turner,* Paul M. Johns, Evan M. Thatcher, D. B. Tanner, and Juan C. Nino

28804  DOI: 10.1021/jp5096129

Morphological Tunability of the Plasmonic Response: From Hollow Gold Nanoparticles to Gold Nanorings

Martin Prieto, Raul Arenal,* Luc Henrard, Leyre Gomez, Victor Sebastian, and Manuel Arruebo*

28812  DOI: 10.1021/jp509666x

Nonlinear Scattering and Absorption Effects in Size-Selected Diphenylpolyynes

E. Fazio, L. D'Urso,* G. Consiglio, A. Giuffrida, G. Compagnini, O. Puglisi, S. Patanè, F. Neri, and G. Forte

28820  DOI: 10.1021/jp510105z

Photobleaching of Fluorophores on the Surface of Nanoantennas

C. M. Galloway, C. Artur, J. Grand, and E. C. Le Ru*

28831  DOI: 10.1021/jp510581m

Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes

Titouan Jaunet-Lahary, Agisilaos Chantzis,* Kathy J. Chen, Adèle D. Laurent, and Denis Jacquemin*

Physical Processes in Nanomaterials and Nanostructures

28842  DOI: 10.1021/jp509011u

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H. Yamagata, D. S. Maxwell, J. Fan, K. R. Kittilstved, A. L. Briseno, M. D. Barnes, and F. C. Spano*

28855  DOI: 10.1021/jp5092077

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Anna P. Goldstein, William Mickelson, Ariella Machness, Gloria Lee, Marcus A. Worsley, Leta Woo, and Alex Zettl*

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DOI: 10.1021/jp509264a

Surface Reconstruction and Reactivity of Platinum–Iron Oxide Nanoparticles

Paul N. Duchesne, Guangxu Chen, Xiaojing Zhao, Nanfeng Zheng, and Peng Zhang*

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DOI: 10.1021/jp509437a

Impact of the AuAg NPs Composition on Their Structure and Properties: A Theoretical and Experimental Investigation

Janaina F. Gomes,* Amanda C. Garcia, Cleiton Pires, Eduardo B. Ferreira, Rodrigo Q. Albuquerque,* Germano Tremiliosi-Filho, and Luiz H. S. Gasparotto

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DOI: 10.1021/jp509849a

Aberration Corrected Electron Microscopy Study of Bimetallic Pd–Pt Nanocrystal: Core–Shell Cubic and Core–Frame Concave Structures

Ning Lu, Jinguo Wang, Shuifen Xie, Jacob Brink, Kevin McIlwrath, Younan Xia, and Moon J. Kim*

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DOI: 10.1021/jp509975w

Facile Synthesis of an Extensive Family of $\text{Sc}_2\text{O}@\text{C}_{2n}$ ($n = 35\text{--}47$) and Chemical Insight into the Smallest Member of $\text{Sc}_2\text{O}@\text{C}_2(7892)\text{--}\text{C}_{70}$

Meirong Zhang, Yajuan Hao, Xiaohong Li, Lai Feng,* Ting Yang, Yingbo Wan, Ning Chen,* Zdeněk Slanina,* Filip Uhlík, and Hailin Cong*

28890 

DOI: 10.1021/jp509978j

Low-Temperature ^{23}Na MAS NMR Reveals Dynamic Effects and Compositions for the Large and Small Channels in the Zeolite-Like Ge-Framework of $\text{Na}_{1-x}\text{Ge}_{3+x}$ Materials

Hans J. Jakobsen,* Henrik Bildsøe, Matt Beekman, Stevce Stefanoski, George S. Nolas,* and Clifford R. Bowers*

28898 

DOI: 10.1021/jp5101158

Size Quantization Effects on Interfacial Electron Transfer Dynamics in Ru(II)–Polypyridyl Complex Sensitized ZnO QDs

Sandeep Verma,* Amitava Das,* and Hirendra N. Ghosh*

28906 

DOI: 10.1021/jp5102219

Temperature-Dependent Structural Transitions in Methane–Ethane Mixed Gas Hydrates


Minchul Kwon, Jong-Won Lee,* and Huen Lee*

28914

DOI: 10.1021/jp510229f

Solid-State NMR Study of Hydroxyapatite Containing Amorphous Phosphate Phase and Nanostructured Hydroxyapatite: Cut-Off Averaging of CP-MAS Kinetics and Size Profiles of Spin Clusters

Vytautas Klimavicius, Aivaras Kareiva, and Vytautas Balevicius*

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