

January 10, 2013 Volume 117, Issue 1

Pages 1-728

Sample This sample issue provides free access to the full text of all articles. (Subscription Information)

Editorial

Editorial for January 2013 for JPC A/B/C

Anne B. McCoy, Sharon Hammes-Schiffer, Catherine J. Murphy, and George C. Schatz pp 1–2

Publication Date (Web): January 10, 2013 (Editorial)

DOI: 10.1021/jp311639f

Energy Conversion and Storage; Energy and Charge Transport

Effect of Transition Metal Dopants on Initial Mass Transport in the Dehydrogenation of NaAlH₄: Density Functional Theory Study

Ali Marashdeh, Jan-Willem I. Versluis, Álvaro Valdés, Roar A. Olsen, Ole Martin Løvvik, and Geert-Jan Kroes

pp 3–14

Publication Date (Web): November 27, 2012 (Article)

DOI: 10.1021/jp301199e

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Theoretical Approach to the Study of Thiophene-Based Discotic Systems As Organic Semiconductors

Gregorio García, Mónica Moral, José M. Granadino-Roldán, Andrés Garzón, Amparo Navarro, and Manuel Fernández-Gómez

pp 15–22

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp304952y

Section:

Physical Organic Chemistry

First-Principles Study on the Synergistic Mechanism of SnO₂ and Graphene As a Lithium Ion Battery Anode

Ling Miao, Jiangbin Wu, Jianjun Jiang, and Pei Liang

pp 23–27

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp306572c

Section:

Electric Phenomena

Mesoscale Phase-Field Modeling of Charge Transport in Nanocomposite Electrodes for Lithium-Ion Batteries

Shenyang Hu, Yulan Li, Kevin M. Rosso, and Maria L. Sushko pp 28–40

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp3068014

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Effective Reversible Potentials and Onset Potentials for O₂ Electroreduction on Transition Metal Electrodes: Theoretical Analysis

Alfred B. Anderson, Ryosuke Jinnouchi, and Jamal Uddin pp 41–48

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp307367m

Section: Electrochemistry

Optimization of a High Work Function Solution Processed Vanadium Oxide Hole-Extracting Layer for Small Molecule and Polymer Organic Photovoltaic Cells

I. Hancox, L. A. Rochford, D. Clare, M. Walker, J. J. Mudd, P. Sullivan, S. Schumann, C. F. McConville, and T. S. Jones

pp 49–57

Publication Date (Web): November 27, 2012 (Article)

DOI: 10.1021/jp3075767

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Co-Actions of Ambient Pressure and Gas Molecular Adsorption on the Carriers' Transport in Polycrystalline Pentacene Thin-Film Transistors

Haoyan Zhao, Guifang Dong, Lian Duan, Liduo Wang, and Yong Qiu pp 58–63

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp308088b

Section:

Electric Phenomena

Ultrafast Energy Transfer in Divinylbiphenyl and Divinylstilbene Copolymers Bridged by Silylene

Kuan-Lin Liu, Sheng-Jui Lee, and I-Chia Chen , Chao-Ping Hsu , Chih-Hsien Chen and Tien-Yau Luh

pp 64–70

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp3082003

Section:

Physical Properties of Synthetic High Polymers

Interpenetration of Metal Organic Frameworks for Carbon Dioxide Capture and Hydrogen Purification: Good or Bad?

Sang Soo Han, Dong-Hyun Jung, and Jiyoung Heo

pp 71–77

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp308751x

Section:

Surface Chemistry and Colloids

Physicochemical Properties of Binary Ionic Liquid–Aprotic Solvent Electrolyte Mixtures

Eric T. Fox, Elie Paillard, Oleg Borodin, and Wesley A. Henderson

pp 78–84

Publication Date (Web): November 29, 2012 (Article)

DOI: 10.1021/jp3089403

Section:

Physical Organic Chemistry

Effect of Plasmonic Au Nanoparticles on Inverted Organic Solar Cell Performance

Jian Wang, Yun-Ju Lee, Arvinder S. Chadha, Juan Yi, Michael L. Jespersen, John J. Kelley, Hue M. Nguyen, Michael Nimmo, Anton V. Malko, Richard A. Vaia, Weidong Zhou, and Julia W. P. Hsu

pp 85–91

Publication Date (Web): November 26, 2012 (Article)

DOI: 10.1021/jp309415u

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Significantly Enhanced Open Circuit Voltage and Fill Factor of Quantum Dot Sensitized Solar Cells by Linker Seeding Chemical Bath Deposition

Keyou Yan, Wei Chen, and Shihe Yang pp 92–99

Publication Date (Web): December 7, 2012 (Article)

DOI: 10.1021/jp3094319

Section:

Electrochemical, Radiational, and Thermal Energy Technology

First-Principles Study of Multiterminal Quantum Interference Controlled Molecular Devices

Yukihiro Okuno and Taisuke Ozaki

pp 100-109

Publication Date (Web): December 14, 2012 (Article)

DOI: 10.1021/jp309455n

Section:

Electric Phenomena

Charge Injection Rates in Hybrid Nanosilicon-Polythiophene Bulk Heterojunction Solar Cells

Alexandra Carvalho, Natalia Martsinovich, Ricardo Vieira, and Alessandro Troisi pp 110–115

Publication Date (Web): December 4, 2012 (Article)

DOI: 10.1021/jp3095825

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Observation of Multiexponential Pico- to Subnanosecond Electron Injection in Optimized Dye-Sensitized Solar Cells with Visible-Pump Mid-Infrared-Probe Transient Absorption Spectroscopy

Mindaugas Juozapavicius, Marius Kaucikas, Jasper J. van Thor, and Brian C. O'Regan pp 116–123

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp309732z

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Reverse Switching Phenomena in Hybrid Organic–Inorganic Thin Film Composite Material

Kallol Mohanta, Jose Rivas, and Ranjith Krishna Pai

pp 124–130

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp309750p

Section:

Electric Phenomena

P3HT/PCBM Photoactive Materials for Solar Cells: Morphology and Dynamics by Means of Solid-State NMR

Francesca Martini, Silvia Borsacchi, Silvia Spera, Chiara Carbonera, Alessandra Cominetti, and Marco Geppi pp 131–139

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp3103904

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Stochastic Resonance in a Molecular Redox Circuit

Yoshiaki Hirano, Yuji Segawa, Tomoji Kawai, and Takuya Matsumoto pp 140–145

Publication Date (Web): December 6, 2012 (Article)

DOI: 10.1021/jp310486z

Section: Electric Phenomena

Strain Modulation of Defect Structure in Gadolinia-Doped Ceria

Bu Wang and Alastair N. Cormack

pp 146–151

Publication Date (Web): December 6, 2012 (Article)

DOI: 10.1021/jp310518j

Section:

Crystallography and Liquid Crystals

Pressure-Induced Irreversible Phase Transition in the Energetic Material Urea Nitrate: Combined Raman Scattering and X-ray Diffraction Study

Shourui Li, Qian Li, Kai Wang, Mi Zhou, Xiaoli Huang, Jing Liu, Ke Yang, Bingbing Liu, Tian Cui, Guangtian Zou, and Bo Zou pp 152–159

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp311208c

Section:

Surfaces, Interfaces, Porous Materials, and Catalysis

Structural Characterization of a Manganese Oxide Barrier Layer Formed by Chemical Vapor Deposition for Advanced Interconnects Application on SiOC Dielectric Substrates

Nguyen Mai Phuong, Yuji Sutou, and Junichi Koike pp 160–164

Publication Date (Web): November 27, 2012 (Article)

DOI: 10.1021/jp303241c

Section: Electric Phenomena

Water Growth on GeO₂/Ge(100) Stack and Its Effect on the Electronic Properties of GeO₂

Atsushi Mura, Iori Hideshima, Zhi Liu, Takuji Hosoi, Heiji Watanabe, and Kenta Arima pp 165–171

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp304331c

Section:

Electric Phenomena

Comparative Study of the Passivation of Al(111) by Molecular Oxygen and Water Vapor

Na Cai and Guangwen Zhou , Kathrin Müller and David E. Starr pp 172–178

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp305740s

Section:

Surface Chemistry and Colloids

Tomography and High-Resolution Electron Microscopy Study of Surfaces and Porosity in a Plate-like γ -Al₂O₃

Libor Kovarik, Arda Genc, Chongmin Wang, Annie Qiu, Charles H. F. Peden, János Szanyi, and Ja Hun Kwak

pp 179-186

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp306800h

Section:

First-Principles Study of the Interfaces between Fe and Transition Metal Carbides

Na-Young Park, Jung-Hae Choi, Pil-Ryung Cha, Woo-Sang Jung, Soon-Hyo Chung, and Seung-Cheol Lee

pp 187–193

Publication Date (Web): November 19, 2012 (Article)

DOI: 10.1021/jp306859n

Section:

Surface Chemistry and Colloids

Analysis of H₂ Release from Organic Polycyclics over Pd Catalysts Using DFT

Farnaz Sotoodeh and Kevin J. Smith

pp 194-204

Publication Date (Web): November 27, 2012 (Article)

DOI: 10.1021/jp307325s

Section:

Physical Organic Chemistry

Electric Double Layer of Au(100)/Imidazolium-Based Ionic Liquids Interface: Effect of Cation Size

Yuzhuan Su, Jiawei Yan, Miangang Li, Meng Zhang, and Bingwei Mao pp 205–212

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp3079919

Section:

Surface Chemistry and Colloids

Ecofriendly Synthesis and Photocatalytic Activity of Uniform Cubic Ag@AgCl Plasmonic Photocatalyst

Rongfang Dong, Baozhu Tian, Cuiyun Zeng, Taoyun Li, Tingting Wang, and Jinlong Zhang pp 213–220

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp311970k

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Growth and Morphology of Ceria on Ruthenium (0001)

B. Kaemena, S. D. Senanayake, A. Meyer, J. T. Sadowski, J. Falta, and J. I. Flege pp 221–232

Publication Date (Web): December 4, 2012 (Article)

DOI: 10.1021/jp3081782

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Beveled Oxide Study of the Surface Potential Modulation of Self Assembled Alkyltrichlorosilanes

Lior Kornblum, Yair Paska, Hossam Haick, and Moshe Eizenberg pp 233–237

Publication Date (Web): December 19, 2012 (Article)

DOI: 10.1021/jp308312m

Section:

Surface Chemistry and Colloids

Desorption/Ionization Efficiency of Common Amino Acids in Surface-Assisted Laser Desorption/Ionization Mass Spectrometry (SALDI-MS) with Nanostructured Platinum

Syuhei Nitta, Hideya Kawasaki, Takashi Suganuma, Yasushi Shigeri, and Ryuichi Arakawa pp 238–245

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp308380z

Section:

Biochemical Methods

Quantitative Characterization of Hexagonal Packings in Nanoporous Alumina Arrays: A Case Study

José R. Borba, Carolina Brito, Pedro Migowski, Tiberio B. Vale, Daniel A. Stariolo, Sérgio R. Teixeira, and Adriano F. Feil pp 246–251

Publication Date (Web): December 4, 2012 (Article)

DOI: 10.1021/jp308542d

Section:

Surface Chemistry and Colloids

Au Clusters on $TiO_2(110)$ (1 × 1) and (1 × 2) Surfaces Examined by Polarization-Dependent Total Reflection Fluorescence XAFS

Wang-Jae Chun, Kotaro Miyazaki, Naoki Watanabe, Yuichiro Koike, Satoru Takakusagi, Keisuke Fujikawa, Masaharu Nomura, Yasuhiro Iwasawa, and Kiyotaka Asakura pp 252–257

Publication Date (Web): December 5, 2012 (Article)

DOI: 10.1021/jp308567e

Section:

Oxygen Interactions with Silica Surfaces: Coupled Cluster and Density Functional Investigation and the Development of a New ReaxFF Potential

Anant D. Kulkarni, Donald G. Truhlar, Sriram Goverapet Srinivasan, Adri C. T. van Duin, Paul Norman, and Thomas E. Schwartzentruber

pp 258-269

Publication Date (Web): December 4, 2012 (Article)

DOI: 10.1021/jp3086649

Section:

Surface Chemistry and Colloids

Substituent Effect on the Intermolecular Arrangements of One-Dimensional Molecular Assembly on the Si(100)-(2×1)-H Surface

Md. Zakir Hossain, R. S. Dasanayake-Aluthge, Taketoshi Minato, Hiroyuki S. Kato, and Maki Kawai

pp 270-275

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp308770t

Section:

Surface Chemistry and Colloids

Carbon Coating of LiFePO₄ Can Be Strengthened by Sc and Ti

W. T. Geng, T. Ohno

pp 276-279

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp308903v

Section:

Electrochemical, Radiational, and Thermal Energy Technology

NiO-MgO and CoO-MgO Thin-Film Solid Oxide Solutions on a Mo(100) Support: Formation, Reduction, and Influence of the Support

Kathrin Müller, Daniel Torres, Joon B. Park, Ping Liu, Dario Stacchiola, and David E. Starr pp 280–287

Publication Date (Web): December 6, 2012 (Article)

DOI: 10.1021/jp308955n

Section:

Water Oxidation on MnO_x and IrO_x : Why Similar Performance?

Michael Busch, Elisabet Ahlberg, and Itai Panas pp 288–292

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp308982s

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Theoretical Study of the Structures and Chemical Ordering of Palladium–Gold Nanoalloys Supported on MgO(100)

Ramli Ismail, Riccardo Ferrando, and Roy L. Johnston pp 293–301

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp3093435

Section:

Surface Chemistry and Colloids

Molecular Multistate Systems Formed in Two-Dimensional Porous Networks on Ag(111)

Kyung-Hoon Chung, Howon Kim, Won Jun Jang, Jong Keon Yoon, Se-Jong Kahng, Jhinhwan Lee, and Seungwu Han pp 302–306

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp309554z

Section:

Surface Chemistry and Colloids

Triphenylene Substituted Pyrene Derivative: Synthesis and Single Molecule Investigation

Xue-mei Zhang, Hai-feng Wang, Shuai Wang, Yong-tao Shen, Yan-lian Yang, Ke Deng, Keqing Zhao, Qing-dao Zeng, and Chen Wang pp 307–312

Publication Date (Web): November 30, 2012 (Article)

DOI: 10.1021/jp3095616

Section:

Benzene, Its Derivatives, and Condensed Benzenoid Compounds

Influence of Hole-Sequestering Ligands on the Photostability of CdSe Quantum Dots

Yizheng Tan, Song Jin, and Robert J. Hamers

pp 313-320

Publication Date (Web): December 14, 2012 (Article)

DOI: 10.1021/jp309587k

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

van der Waals-Corrected Ab Initio Study of Water Ice— Graphite Interaction

Alberto Ambrosetti , Francesco Ancilotto and Pier Luigi Silvestrelli

pp 321-325

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp309617f

Section:

Physical Organic Chemistry

Thermal Decomposition of Silver Carbonate: Phenomenology and Physicogeometrical Kinetics

Nobuyoshi Koga, Shuto Yamada, and Tomoyasu Kimura

pp 326-336

Publication Date (Web): December 6, 2012 (Article)

DOI: 10.1021/jp309655s

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Adsorption of Methanethiolate and Atomic Sulfur at the Cu(111) Surface: A Computational Study

Porntip Seema, Jörg Behler, and Dominik Marx

pp 337–348

Publication Date (Web): December 14, 2012 (Article)

DOI: 10.1021/jp309728w

Section:

Surface Chemistry and Colloids

A Grand-Canonical Monte Carlo Study of the Adsorption Properties of Argon Confined in ZIF-8: Local Thermodynamic Modeling

Federico G. Pazzona, Pierfranco Demontis, and Giuseppe B. Suffritti pp 349–357

Publication Date (Web): December 4, 2012 (Article)

DOI: 10.1021/jp309797j

Section:

DFT Simulations of Titanium Oxide Films on Titanium Metal

Bastian Ohler, Stefano Prada, Gianfranco Pacchioni, and Walter Langel pp 358–367

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp309827u

Section:

Surface Chemistry and Colloids

Functionalization of Azide-Terminated Silicon Surfaces with Glycans Using Click Chemistry: XPS and FTIR Study

A. C. Gouget-Laemmel, J. Yang, M. A. Lodhi, A. Siriwardena, D. Aureau, R. Boukherroub, J.-N. Chazalviel, F. Ozanam, and S. Szunerits pp 368–375

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp309866d

Sulfurization-Assisted Cobalt Deposition on Sm₂Ti₂S₂O₅ Photocatalyst for Water Oxidation under Visible Light Irradiation

Rengui Li, Zheng Chen, Wen Zhao, Fuxiang Zhang, Kazuhiko Maeda, Baokun Huang, Shuai Shen, Kazunari Domen, and Can Li pp 376–382

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp310138b

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Physicochemical Origin for Free Radical Generation of Iron Oxide Nanoparticles in Biomicroenvironment: Catalytic Activities Mediated by Surface Chemical States

Bing Wang, Jun-Jie Yin, Xiaoyan Zhou, Ibrahim Kurash, Zhifang Chai, Yuliang Zhao, and Weiyue Feng

pp 383-392

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp3101392

Section: Pharmaceuticals

Noble Gas Separation using PG-ESX (X = 1, 2, 3)Nanoporous Two-Dimensional Polymers

Anna M. Brockway and Joshua Schrier

pp 393-402

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp3101865

Section:

Surface Chemistry and Colloids

Densification of C–S–H Measured by ¹H NMR Relaxometry

Arnaud C. A. Muller, Karen L. Scrivener, Agata M. Gajewicz, and Peter J. McDonald pp 403–412

Publication Date (Web): December 7, 2012 (Article)

DOI: 10.1021/jp3102964

Section:

Cement, Concrete, and Related Building Materials

Stability of Extraframework Iron-Containing Complexes in ZSM-5 Zeolite

Guanna Li, Evgeny A. Pidko, Rutger A. van Santen, Can Li, and Emiel J. M. Hensen pp 413–426

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp310374k

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Effects of Localized Surface Charges on a Two-Dimensional Potential Distribution and Photovoltage at a Schottky Barrier of a Semiconductor Electrode

Yoshihiro Nakato pp 427–432

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp3104408

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Computational Investigation of CO Adsorption and Oxidation on Mn/CeO₂(111) Surface

Ling-Chieh Hsu, Ming-Kang Tsai, Yu-Huan Lu, and Hsin-Tsung Chen pp 433–441

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp310457g

Section:

Reaction Mechanism of Selective Photooxidation of Amines over Niobium Oxide: Visible-Light-Induced Electron Transfer between Adsorbed Amine and Nb₂O₅

Shinya Furukawa, Yasuhiro Ohno, Tetsuya Shishido, Kentaro Teramura, and Tsunehiro Tanaka pp 442–450

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp310501h

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Influence of Step Defects on Methanol Decomposition: Periodic Density Functional Studies on Pd(211) and Kinetic Monte Carlo Simulations

Sen Lin, Jianyi Ma, Linsen Zhou, Caijin Huang, Daiqian Xie, and Hua Guo pp 451–459

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp310600q

Section:

Surface Chemistry and Colloids

Electronic Origin of the Surface Reactivity of Transition-Metal-Doped $TiO_2(110)$

Mónica García-Mota, Aleksandra Vojvodic, Frank Abild-Pedersen, and Jens K. Nørskov pp 460–465

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp310667r

Section:

General Physical Chemistry

Toward a Transferable Set of Charges to Model Zeolitic Imidazolate Frameworks: Combined Experimental—Theoretical Research

Juan José Gutiérrez Sevillano, Sofia Calero, Conchi O. Ania, José B. Parra, Freek Kapteijn, Jorge Gascon, and Said Hamad

pp 466–471

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp3107167

Section:

Horizontal Attenuated Total Reflectance Fourier Transform Infrared and X-ray Photoelectron Spectroscopy Measurements of Water Adsorption on Oxidized Tin(II) Sulfide (SnS) Surfaces

Courtney D. Hatch, Matthew J. Christie, Robert M. Weingold, Chia-Ming Wu, David M. Cwiertny, and Jonas Baltrusaitis

pp 472–482

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp310726t

Section:

Surface Chemistry and Colloids

Au-Decorated Silicene: Design of a High-Activity Catalyst toward CO Oxidation

Chong Li, Shengxue Yang, Shu-Shen Li, Jian-Bai Xia, and Jingbo Li pp 483–488

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp310746m

Section:

Air Pollution and Industrial Hygiene

Double-Shelled Yolk-Shell Microspheres with Fe₃O₄ Cores and SnO₂ Double Shells as High-Performance Microwave Absorbers

Jiwei Liu, Jin Cheng, Renchao Che, Junjie Xu, Mengmei Liu, and Zhengwang Liu pp 489–495

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp310898z

Section:

Electric Phenomena

Nano-nitride Cathode Catalysts of Ti, Ta, and Nb for Polymer Electrolyte Fuel Cells: Temperature-Programmed Desorption Investigation of Molecularly Adsorbed Oxygen at Low Temperature

Ryohji Ohnishi, Kazuhiro Takanabe, Masao Katayama, Jun Kubota, and Kazunari Domen pp 496–502

Publication Date (Web): December 12, 2012 (Article)

DOI: 10.1021/jp3109573

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Development and Optimization of a New Force Field for Flexible Aluminosilicates, Enabling Fast Molecular Dynamics Simulations on Parallel Architectures

Andrea Gabrieli, Marco Sant, Pierfranco Demontis, and Giuseppe B. Suffritti pp 503–509

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp311411b

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Enhanced Autoionization of Water at Phospholipid Interfaces

Alireza Mashaghi, P. Partovi-Azar, Tayebeh Jadidi, Mehrnaz Anvari, Sara Panahian Jand, Nasser Nafari, M. Reza Rahimi Tabar, Philipp Maass, Huib J. Bakker, and Mischa Bonn pp 510–514

Publication Date (Web): December 31, 2012 (Article)

DOI: 10.1021/jp3119617

Section:

Surface Chemistry and Colloids

Plasmonics, Optical Materials, and Hard Matter

Chirality Dependence of Electron Transport Properties of Single-Walled GeC Nanotubes

Pabitra Narayan Samanta and Kalyan Kumar Das pp 515–521

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp306526b

Section:

Electric Phenomena

Kinetic Analysis of O₂- and NO₂-Based Oxidation of Synthetic Soot

C. Wang-Hansen, S. Soltani, and B. Andersson pp 522–531

Publication Date (Web): December 3, 2012 (Article)

DOI: 10.1021/jp307789r

Section:

Air Pollution and Industrial Hygiene

Photo- and Electroluminescence from 2-(Dibenzo[b,d]furan-4-yl)pyridine-Based Heteroleptic Cyclometalated

Platinum(II) Complexes: Excimer Formation Drastically Facilitated by an Aromatic Diketonate Ancillary Ligand

Tatsuya Shigehiro, Shigeyuki Yagi, Takeshi Maeda, Hiroyuki Nakazumi, Hideki Fujiwara, and Yoshiaki Sakurai

pp 532-542

Publication Date (Web): November 10, 2012 (Article)

DOI: 10.1021/jp307853t

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Study of Ultraviolet Emission Enhancement in Al_xIn_yGa_{1-x-}_yN Quaternary Alloy Film

Dongbo Wang, Shujie Jiao, Liancheng Zhao, Tong Liu, Shiyong Gao, Hongtao Li, Jinzhong Wang, Qingjiang Yu, and Fengyun Guo pp 543–548

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp3088429

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Extension of Molecular Structure toward Solution-Processable Hosts for Efficient Blue Phosphorescent Organic Light-Emitting Diodes

Shaolong Gong, Cheng Zhong, Qiang Fu, Dongge Ma, Jingui Qin, and Chuluo Yang pp 549–555

Publication Date (Web): December 24, 2012 (Article)

DOI: 10.1021/jp309100e

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Exploring the Chemical Enhancement of Surface-Enhanced Raman Scattering with a Designed Silver/Silica Cavity Substrate

Shu Tian, Qun Zhou, Chuanhong Li, Zhuomin Gu, John R. Lombardi, and Junwei Zheng pp 556–563

Publication Date (Web): December 18, 2012 (Article)

DOI: 10.1021/jp309224m

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Highly Efficient Construction of Silver Nanosphere Dimers on Poly(dimethylsiloxane) Sheets for Surface-Enhanced Raman Scattering

Hongyun Guo, Dan Jiang, Haibo Li, Shuping Xu, and Weiqing Xu pp 564–570

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp309396x

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Galvanic Exchange on Reduced Graphene Oxide: Designing a Multifunctional Two-Dimensional Catalyst Assembly

Sachidananda Krishnamurthy and Prashant V. Kamat

pp 571-577

Publication Date (Web): November 27, 2012 (Article)

DOI: 10.1021/jp309529b

Section: Electrochemistry

Stimulating Multiple SERS Mechanisms by a Nanofibrous Three-Dimensional Network Structure of Titanium Dioxide (TiO₂)

Dmitry Maznichenko, Krishnan Venkatakrishnan, and Bo Tan pp 578–583

Publication Date (Web): December 3, 2012 (Article)

DOI: 10.1021/jp310193a

Section:

Biochemical Methods

Local Dielectric Environment Dependent Local Electric Field Enhancement in Double Concentric Silver Nanotubes

Jian Zhu, Jian-Jun Li, and Jun-Wu Zhao

pp 584-592

Publication Date (Web): December 14, 2012 (Article)

DOI: 10.1021/jp310676s

Section:

Electric Phenomena

Physical Processes in Nanomaterials and Nanostructures

Effect of Reductive Dithiothreitol and Trolox on Nitric Oxide Quenching of Single-Walled Carbon Nanotubes

Selda Sen, Fatih Sen, Ardemis A. Boghossian, Jingqing Zhang, and Michael S. Strano pp 593–602

Publication Date (Web): November 15, 2012 (Article)

DOI: 10.1021/jp307175f

Section:

Biochemical Methods

Thio-Mayan-like Compounds: Excited State Characterization of Indigo Sulfur Derivatives in Solution and Incorporated in Palygorskite and Sepiolite Clays

Raquel Rondão and J. Sérgio Seixas de Melo

pp 603–614

Publication Date (Web): December 6, 2012 (Article)

DOI: 10.1021/jp306209y

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

High-Pressure Behaviors of SrF₂ Nanocrystals with Two Morphologies

Jingshu Wang, Hongyang Zhu, Chunli Ma, Xiaoxin Wu, Jian Zhang, Dongmei Li, Ridong Cong, Jing Liu, and Qiliang Cui

pp 615-619

Publication Date (Web): December 10, 2012 (Article)

DOI: 10.1021/jp306742p

Section:

Crystallography and Liquid Crystals

Use of Optical Contrast To Estimate the Degree of Reduction of Graphene Oxide

Francesco Perrozzi, Stefano Prezioso, Maurizio Donarelli, Federico Bisti, Patrizia De Marco, Sandro Santucci, Michele Nardone, Emanuele Treossi, Vincenzo Palermo, and Luca Ottaviano pp 620–625

Publication Date (Web): December 3, 2012 (Article)

DOI: 10.1021/jp3069738

Section:

Electric Phenomena

Linear and Nonlinear Optical Properties of Ramified Hexaazatriphenylenes: Charge Transfer Contributions to the Octupolar Response

María Moreno Oliva, Rafael Juárez, Mar Ramos, José L. Segura, Stijn van Cleuvenbergen, Koen Clays, Theodore Goodson, III, Juan T. López Navarrete, and Juan Casado pp 626–632

Publication Date (Web): December 5, 2012 (Article)

DOI: 10.1021/jp307563u

Section:

Physical Organic Chemistry

Electronic and Magnetic Changes in a Finite-Sized Single-Walled Zigzag Carbon Nanotube Embedded in Water

Carlos M. Ruiz and Sergio D. Dalosto

pp 633-638

Publication Date (Web): December 12, 2012 (Article)

DOI: 10.1021/jp308174k

Section:

Electric Phenomena

Pressure-Induced Fluorescence Enhancement of the BSA-Protected Gold Nanoclusters and the Corresponding Conformational Changes of Protein

Min Zhang, Yong-Qiang Dang, Tian-Ying Liu, Hong-Wei Li, Yuqing Wu, Qian Li, Kai Wang, and Bo Zou pp 639–647

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp309175k

Section:

General Biochemistry

Study of the Partial Ag-to-Zn Cation Exchange in AgInS₂/ZnS Nanocrystals

Baodong Mao, Chi-Hung Chuang, Feng Lu, Lixia Sang, Junjie Zhu, and Clemens Burda pp 648–656

Publication Date (Web): December 24, 2012 (Article)

DOI: 10.1021/jp309202g

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Multiphonon Raman Scattering in Coupled Cd_{1-x}Mn_xS Nanoparticles: Magnetic Doping and Thermal Annealing

Ernesto S. Freitas Neto, Sebastião W. da Silva, Paulo C. Morais, and Noelio O. Dantas pp 657–662

Publication Date (Web): December 15, 2012 (Article)

DOI: 10.1021/jp309270t

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Laser-Assisted Simultaneous Patterning and Transferring of Graphene

Joon-Suk Oh, Sang-Hoon Kim, Taeseon Hwang, Hyuk-Yong Kwon, Tae Hee Lee, Ah-Hyun Bae, Hyouk Ryeol Choi, and Jae-Do Nam

pp 663–668

Publication Date (Web): December 11, 2012 (Article)

DOI: 10.1021/jp309382w

Section:

Electric Phenomena

Oligonucleotide Functionalization of Hollow Triangular **Gold Silver Alloy Nanoboxes**

Gemma L. Keegan, Damian Aherne, Eric Defrancq, Yurii K. Gun'ko, and John M. Kelly pp 669–676

Publication Date (Web): December 4, 2012 (Article)

DOI: 10.1021/jp309449d

Section:

Nonferrous Metals and Alloys

Dependencies of Donor-Acceptor Memory on Molecular Levels

Raymond Sim, Wang Ming, Yudi Setiawan, and Pooi See Lee pp 677–682

Publication Date (Web): December 20, 2012 (Article)

DOI: 10.1021/jp309456y

Section:

Electric Phenomena

Precise Control of the Number of Walls of Carbon Nanotubes of a Uniform Internal Diameter

Ankur Baliyan, Yasuhiro Hayasaki, Takahiro Fukuda, Takashi Uchida, Yoshikata Nakajima, Tatsuro Hanajiri, and Toru Maekawa

pp 683-686

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp309894s

Section:

Industrial Inorganic Chemicals

Substrate-Driven Formation of Bidimensional Arrays of Co Nanocrystals in TiO₂ Thin Films

Tian Li, Rosanna Larciprete, Stefano Turchini, Nicola Zema, Alberta Bonanni, and Antonio Di Trolio

pp 687-691

Publication Date (Web): December 13, 2012 (Article)

DOI: 10.1021/jp309953h

Section:

Surface Chemistry and Colloids

Electronic and Field Emission Properties of Wrinkled Graphene

Yufeng Guo and Wanlin Guo

pp 692-696

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp3103063

Section:

Electric Phenomena

Synthesis of Homogeneous Manganese-Doped Titanium Oxide Nanotubes from Titanate Precursors

Péter Szirmai, Endre Horváth, Bálint Náfrádi, Zlatko Micković, Rita Smajda, Dejan M. Djokić, Kurt Schenk, László Forró, and Arnaud Magrez pp 697–702

Publication Date (Web): December 12, 2012 (Article)

DOI: 10.1021/jp3104722

Section:

Magnetic Phenomena

Controlling Nanoparticle Dynamics in Conical Nanopores

Sean R. German, Long Luo, Henry S. White, and Tony L. Mega pp 703–711

Publication Date (Web): December 3, 2012 (Article)

DOI: 10.1021/jp310513v

Section:

Polymerization of Tetracyanoethylene under Pressure

Mohammad Khazaei, Masao Arai, Taizo Sasaki, and Yoshiyuki Kawazoe pp 712–720

Publication Date (Web): December 17, 2012 (Article)

DOI: 10.1021/jp310747v

Section:

Chemistry of Synthetic High Polymers

Comments

Comment on "How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene"

Panaghiotis Karamanis and Claude Pouchan pp 721–724

Publication Date (Web): December 11, 2012 (Comment)

DOI: 10.1021/jp3057256

Section:

General Physical Chemistry

Reply to "Comment on 'How the Number and Location of Lithium Atoms Affect the First Hyperpolarizability of Graphene"

Yang-Yang Hu, Hong-Liang Xu, and Zhong-Min Su pp 725–728

Publication Date (Web): December 11, 2012 (Comment)

DOI: 10.1021/jp309686h

Section:

General Physical Chemistry