

ПИ
980/pc2

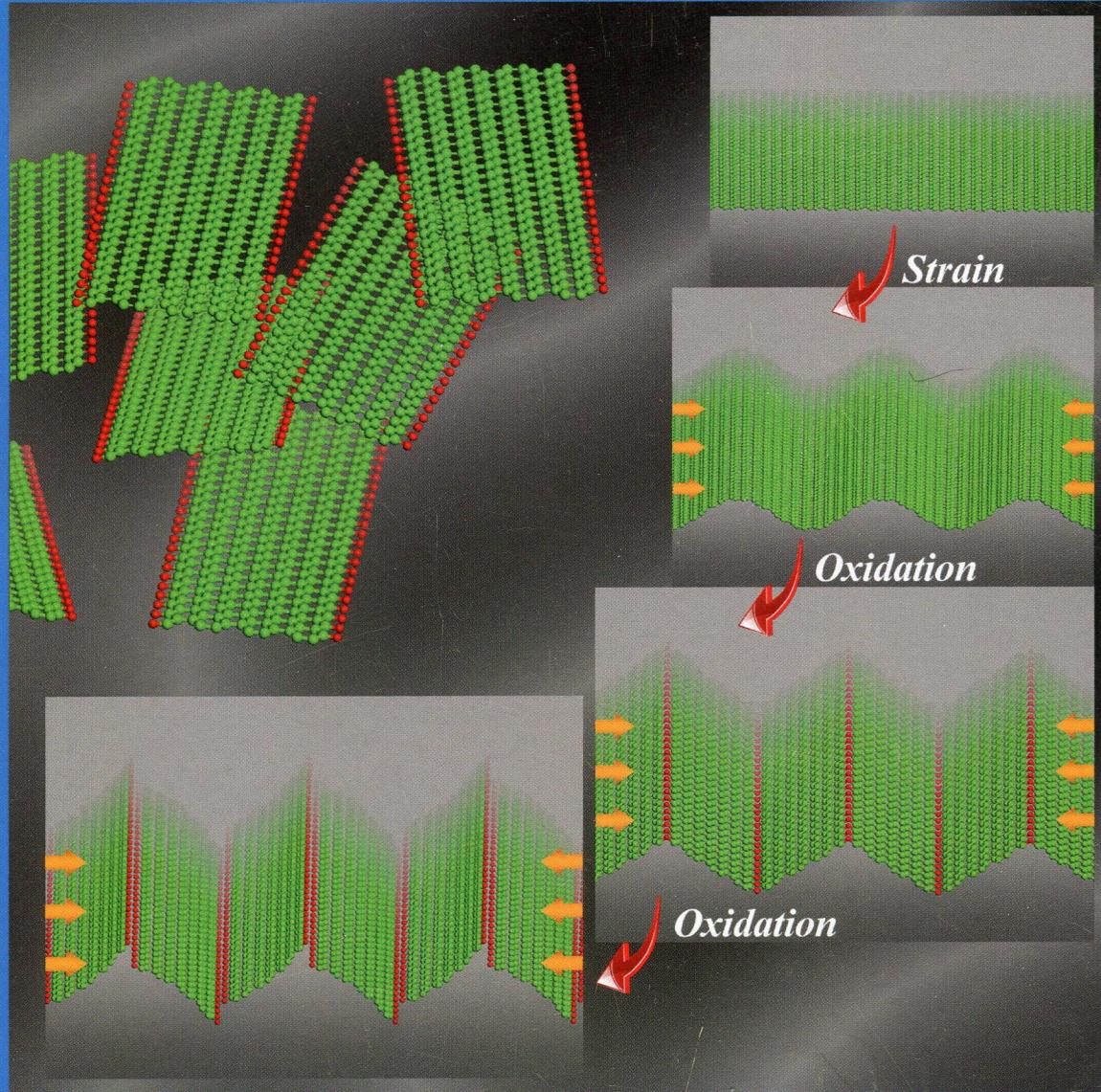
SEPTEMBER 19, 2013

VOLUME 117

NUMBER 37

pubs.acs.org/JPCC

THE JOURNAL OF PHYSICAL CHEMISTRY C



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



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

www.acs.org

THE JOURNAL OF PHYSICAL CHEMISTRY C

September 19, 2013

Volume 117, Issue 37

Pages 18789-19254

Feature Article

Strain Influence on the Oxygen Electrocatalysis of the (100)-Oriented Epitaxial La₂NiO_{4+δ} Thin Films at Elevated Temperatures

Dongkyu Lee, Alexis Grimaud, Ethan J. Crumlin, Khaled Mezghani, Mohamed A. Habib, Zhenxing Feng, Wesley T. Hong, Michael D. Biegalski, Hans M. Christen, and Yang Shao-Horn

pp 18789–18795

Publication Date (Web): August 20, 2013 (Feature Article)

DOI: 10.1021/jp404121p



Section:
Electrochemistry

Energy Conversion and Storage; Energy and Charge Transport Insights into Degradation of Si Anodes from First-Principle Calculations

Jochen Rohrer and Karsten Albe

pp 18796–18803

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp401379d



Section:
Electrochemical, Radiational, and Thermal Energy Technology

Energy Accommodation between Noble Gases and Carbon Nanotubes

Lin Hu and Alan J. H. McGaughey

pp 18804–18808

Publication Date (Web): August 22, 2013 (Article)

DOI: 10.1021/jp404153d



Section:
General Physical Chemistry

Refined Structure Determination of Blue-Emitting Tris(8-hydroxyquinoline) Aluminum(III) (Alq_3) by the Combined Use of Cross-Polarization/Magic-Angle Spinning ^{13}C Solid-State NMR and First-Principles Calculation

Furitsu Suzuki, Tatsuya Fukushima, Masashi Fukuchi, and Hironori Kaji

pp 18809–18817

Publication Date (Web): August 23, 2013 (Article)

DOI: 10.1021/jp404430v



Optical, Electron, and Mass Spectroscopy and Other Related Properties

Investigation of Fluorescence Emission from CdSe Nanorods in PMMA and P3HT/PMMA Films

Lorinc Sarkany, Jenna M. Wasyleko, Santanu Roy, Daniel A. Higgins, Christopher G. Elles, and Viktor Chikan

pp 18818–18828

Publication Date (Web): August 21, 2013 (Article)

DOI: 10.1021/jp404585j



Optical, Electron, and Mass Spectroscopy and Other Related Properties

Investigation of an Intermediate Temperature Molten Lithium Salt Based on Fluorosulfonyl(trifluoromethylsulfonyl)amide as a Solvent-Free Lithium Battery Electrolyte

Keigo Kubota and Hajime Matsumoto

pp 18829–18836

Publication Date (Web): August 16, 2013 (Article)

DOI: 10.1021/jp405068q



Electrochemical, Radiational, and Thermal Energy Technology

Emergence of Oxygen Reduction Activity in Partially Oxidized Tantalum Carbonitrides: Roles of Deposited Carbon for Oxygen-Reduction-Reaction-Site Creation and Surface Electron Conduction

Akimitsu Ishihara, Motoko Tamura, Yoshiro Ohgi, Masashi Matsumoto, Koichi Matsuzawa, Shigenori Mitsushima, Hideto Imai, and Ken-ichiro Ota

pp 18837–18844

Publication Date (Web): August 22, 2013 (Article)

DOI: 10.1021/jp405247m

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Effects of Geometry and Symmetry on Electron Transport through Graphene–Carbon-Chain Junctions

Yao-Jun Dong, Xue-Feng Wang, Ming-Xing Zhai, Jian-Chun Wu, Liping Zhou, Qin Han, and Xue-Mei Wu

pp 18845–18850

Publication Date (Web): August 22, 2013 (Article)

DOI: 10.1021/jp405318b

Section:

Electric Phenomena

Structural Properties and Reversible Deuterium Loading of MgD₂–TiD₂ Nanocomposites

Marine Ponthieu, Fermin Cuevas, Jose Francisco Fernández, Laetitia Laversenne, Florence Porcher, and Michel Latroche

pp 18851–18862

Publication Date (Web): August 21, 2013 (Article)

DOI: 10.1021/jp405803x

Section:

Inorganic Chemicals and Reactions

Determination of Midgap State Energy Levels of an Anatase TiO₂ Nanocrystal Film by Nanosecond Transient Infrared Absorption – Excitation Energy Scanning Spectra

Ming Zhu, Yang Mi, Gangbei Zhu, Deyong Li, Yunpeng Wang, and Yuxiang Weng

pp 18863–18869

Publication Date (Web): August 22, 2013 (Article)

DOI: 10.1021/jp405968f

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Charge Transfer in CdSe Nanocrystal Complexes with an Electroactive Polymer

Megan H. J. Oh, Ming Chen, Chi-Hung Chuang, Gerard J. Wilson, Clemens Burda, Mitchell A. Winnik, and Gregory D. Scholes

pp 18870–18884

Publication Date (Web): August 23, 2013 (Article)

DOI: 10.1021/jp406196a

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Nanocolumnar Germanium Thin Films as a High-Rate Sodium-Ion Battery Anode Material

Paul R. Abel, Yong-Mao Lin, Tania de Souza, Chia-Yun Chou, Asha Gupta, John B. Goodenough, Gyeong S. Hwang, Adam Heller, and C. Buddie Mullins

pp 18885–18890

Publication Date (Web): August 21, 2013 (Article)

DOI: 10.1021/jp407322k

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Surfaces, Interfaces, Porous Materials, and Catalysis

Binding Interaction and Raman Spectra of p-π Conjugated Molecules Containing CH₂/NH₂ Groups Adsorbed on Silver Surfaces: A DFT Study of Wagging Modes

Sha Tao, Li-Juan Yu, Ran Pang, Yi-Fan Huang, De-Yin Wu, and Zhong-Qun Tian

pp 18891–18903

Publication Date (Web): August 21, 2013 (Article)

DOI: 10.1021/jp4042777

Section:

Physical Organic Chemistry

In Situ Ru K-Edge X-ray Absorption Spectroscopy Study of Methanol Oxidation Mechanisms on Model Submonolayer Ru on Pt Nanoparticle Electrocatalyst

Christopher J. Pelliccione, Elena V. Timofeeva, John P. Katsoudas, and Carlo U. Segre

pp 18904–18912

Publication Date (Web): September 4, 2013 (Article)

DOI: 10.1021/jp404342z

Section:

Electrochemistry

Characterization of Interfaces between Graphene Films and Support Substrates by Observation of Lipid Membrane Formation

Kenji Yamazaki, Syunsuke Kunii, and Toshio Ogino

pp 18913–18918

Publication Date (Web): August 27, 2013 (Article)

DOI: 10.1021/jp404458g

Section:

Surface Chemistry and Colloids

Graphene Nucleation Density on Copper: Fundamental Role of Background Pressure

Ivan Vlassiouk, Sergei Smirnov, Murari Regmi, Sumedh P. Surwade, Nishtha Srivastava, Randall Feenstra, Gyula Eres, Chad Parish, Nick Lavrik, Panos Datskos, Sheng Dai, and Pasquale Fulvio

pp 18919–18926

Publication Date (Web): August 21, 2013 (Article)

DOI: 10.1021/jp4047648

Section:

Ceramics

Amino-Acid Adsorption in MFI-Type Zeolites Enabled by the pH-Dependent Ability to Displace Water

Kai Stückenschneider, Juliane Merz, Felix Hanke, Piotr Rozyczko, Victor Milman, and Gerhard Schembecker

pp 18927–18935

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp4048709

Section:

Amino Acids, Peptides, and Proteins

Ni-Doping Effects on Carbon Diffusion and Oxidation over Mo₂C Surfaces

Yonghui Zhao, Shenggang Li, and Yuhan Sun

pp 18936–18946

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp405209c

Section:

Surface Chemistry and Colloids

Colloidal Stability of Gold Nanoparticles Coated with Multithiol-Poly(ethylene glycol) Ligands: Importance of Structural Constraints of the Sulfur Anchoring Groups

Eunkeu Oh, Kimihiro Susumu, Antti J. Mäkinen, Jeffrey R. Deschamps, Alan L. Huston, and Igor L. Medintz

pp 18947–18956

Publication Date (Web): August 13, 2013 (Article)

DOI: 10.1021/jp405265u

Section:

Surface Chemistry and Colloids

Electrodeposition of Pt Nanoparticle Catalysts from H₂Pt(OH)₆ and Their Application in PEM Fuel Cells

Jonathan J. Burk and Steven K. Buratto

pp 18957–18966

Publication Date (Web): August 16, 2013 (Article)

DOI: 10.1021/jp405302x

Section:

Electrochemical, Radiational, and Thermal Energy Technology

Structure of Self-Assembled Monolayers of Partially Fluorinated Alkanethiols with a Fluorocarbon Part of Variable Length on Gold Substrate

Hao Lu, Daniela Zeysing, Martin Kind, Andreas Terfort, and Michael Zharnikov

pp 18967–18979

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp405475h

Section:

Surface Chemistry and Colloids

Sequence-Programmable Multicomponent Multilayers of Nanometer-Sized Tetralactam Macrocycles on Gold Surfaces

Sebastian Richter, Christoph H.-H. Traulsen, Thomas Heinrich, Johannes Poppenberg, Charlene Leppich, Markus Holzweber, Wolfgang E. S. Unger, and Christoph A. Schalley

pp 18980–18985

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp405492v

Section:

Surface Chemistry and Colloids

O₂ Adsorption and Oxidative Activity on Gold-Based Catalysts with and without a Ceria Support

Bo-Tao Teng, Jia-Jian Lang, Xiao-Dong Wen, Ce Zhang, Maohong Fan, and H. Gordon Harris

pp 18986–18993

Publication Date (Web): August 5, 2013 (Article)

DOI: 10.1021/jp4056279

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Electronic Structure Assessment: Combined Density Functional Theory Calculations and Ru L_{2,3}-Edge X-ray Absorption Near-Edge Spectroscopy of Water Oxidation Catalyst

Igor Alperovich, Dooshaye Moonshiram, Javier J. Concepcion, and Yulia Pushkar

pp 18994–19001

Publication Date (Web): August 12, 2013 (Article)

DOI: 10.1021/jp405648h

Section:

General Physical Chemistry

Chromatography and the Hundred Year Mystery of Inorganic Ions at Aqueous Interfaces: First Evidence of the Presence of a Kosmotrope at the Graphite/Electrolyte Solution Interface

Teresa Cecchi

pp 19002–19009

Publication Date (Web): September 9, 2013 (Article)

DOI: 10.1021/jp405702r

Section:

Surface Chemistry and Colloids

Effect of Lattice Motion on Dissociation and Recombination Rates of H₂ on Ni(100) Surface

Wenji Wang and Yi Zhao

pp 19010–19019

Publication Date (Web): September 4, 2013 (Article)

DOI: 10.1021/jp406000f

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Monovalent Cation-Exchanged Natrolites and Their Behavior under Pressure. A Computational Study

Alena Kremleva, Thomas Vogt, and Notker Rösch

pp 19020–19030

Publication Date (Web): September 9, 2013 (Article)

DOI: 10.1021/jp406037c

Section:

Inorganic Chemicals and Reactions

Influence of Merocyanine Molecular Dipole Moments on the Valence Levels in Thin Films and the Interface Energy Level Alignment with Au(111)

Stefan Krause, Matthias Stolte, Frank Würthner, and Norbert Koch

pp 19031–19037

Publication Date (Web): August 8, 2013 (Article)

DOI: 10.1021/jp4060395

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Structure of a Thermoset Polymer near an Alumina Substrate as Studied by Dissipative Particle Dynamics

Gokhan Kacar, Elias A. J. F. Peters, and Gijsbertus de With

pp 19038–19047

Publication Date (Web): August 21, 2013 (Article)

DOI: 10.1021/jp406060t

Section:

Plastics Manufacture and Processing

Comparative Study of Defect Reactivity in Graphene

Pablo A. Denis and Federico Iribarne

pp 19048–19055

Publication Date (Web): August 10, 2013 (Article)

DOI: 10.1021/jp4061945

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

Insights into the Surface Chemistry of Tin Oxide Atomic Layer Deposition from Quantum Chemical Calculations

Jukka T. Tanskanen and Stacey F. Bent

pp 19056–19062

Publication Date (Web): August 26, 2013 (Article)

DOI: 10.1021/jp4063324

Section:

Surface Chemistry and Colloids

Adsorption of Structural and Stereoisomers of Cyclohexanediamine at the Ge(100)-2 × 1 Surface: Geometric Effects in Adsorption on a Semiconductor Surface

Keith T. Wong and Stacey F. Bent

pp 19063–19073

Publication Date (Web): September 5, 2013 (Article)

DOI: 10.1021/jp406423n

Section:

Surface Chemistry and Colloids

Single Turnover Measurements of Nanoparticle Catalysis Analyzed with Dwell Time Correlation Functions and Constrained Mean Dwell Times

Maicol A. Ochoa, Peng Chen, and Roger F. Loring

pp 19074–19081

Publication Date (Web): September 4, 2013 (Article)

DOI: 10.1021/jp4065246

Section:

Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms

X-ray Reflectivity Reveals a Nonmonotonic Ion-Density Profile Perpendicular to the Surface of ErCl₃ Aqueous Solutions

Guangming Luo, Wei Bu, Miroslav Mihaylov, Ivan Kuzmenko, Mark L. Schlossman, and L. Soderholm

pp 19082–19090

Publication Date (Web): September 4, 2013 (Article)

DOI: 10.1021/jp4067247

Section:

Surface Chemistry and Colloids

Composition- and Aspect-Ratio-Dependent Electrocatalytic Performances of One-Dimensional Aligned Pt-Ni Nanostructures

Ping Wu, Hua Zhang, Yingdan Qian, Yaojuan Hu, Hui Zhang, and Chenxin Cai

pp 19091–19100

Publication Date (Web): August 23, 2013 (Article)

DOI: 10.1021/jp4068087

Section:

Electrochemistry

Time-Resolved Infrared Absorption Study of SrTiO₃ Photocatalysts Codoped with Rhodium and Antimony

Koji Furuhashi, Qingxin Jia, Akihiko Kudo, and Hiroshi Onishi

pp 19101–19106

Publication Date (Web): August 28, 2013 (Article)

DOI: 10.1021/jp407040p

Section:

Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

On the Diffusion of Acetonitrile in Nanoscale Amorphous Silica Pores. Understanding Anisotropy and the Effects of Hydrogen Bonding

Cassandra D. Norton and Ward H. Thompson

pp 19107–19114

Publication Date (Web): August 15, 2013 (Article)

DOI: 10.1021/jp407830f

Section:

General Physical Chemistry

Self-Assembled Molecular Wires and Highly Ordered Monolayer: Thiazole on Ge(100)

Jing Hui He, Wei Mao, Jia Qiang Gu, Guo Qin Xu, and Eng Soon Tok

pp 19115–19118

Publication Date (Web): August 24, 2013 (Article)

DOI: 10.1021/jp407996z

Section:

Surface Chemistry and Colloids

***Plasmonics, Optical Materials, and Hard Matter
Mid-Infrared Surface Plasmon Polariton Sensors Resonant with the Vibrational Modes of Phospholipid Layers***

Odetta Limaj, Fausto D'Apuzzo, Alessandra Di Gaspare, Valeria Giliberti, Fabio Domenici, Simona Sennato, Federico Bordi, Stefano Lupi, and Michele Ortolani

pp 19119–19126

Publication Date (Web): August 8, 2013 (Article)

DOI: 10.1021/jp402629g

Section:

Biochemical Methods

Wide-Band Spectral Control of Au Nanoparticle Plasmon Resonances on a Thermally and Chemically Robust Sensing Platform

Chatdanai Lumdee, Bin Feng Yun, and Pieter G. Kik

pp 19127–19133

Publication Date (Web): August 23, 2013 (Article)

DOI: 10.1021/jp4056522

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

High Power Efficiency Yellow Phosphorescent OLEDs by Using New Iridium Complexes with Halogen-Substituted 2-Phenylbenzo[d]thiazole Ligands

Cong Fan, Liping Zhu, Bei Jiang, Yifan Li, Fangchao Zhao, Dongge Ma, Jingui Qin, and Chuluo Yang

pp 19134–19141

Publication Date (Web): August 22, 2013 (Article)

DOI: 10.1021/jp406220c

Section:

Organometallic and Organometalloidal Compounds

Predicting the Surface Plasmon Resonance Wavelength of Gold–Silver Alloy Nanoparticles

Sammy W. Verbruggen, Maarten Keulemans, Johan A. Martens, and Silvia Lenaerts

pp 19142–19145

Publication Date (Web): August 27, 2013 (Article)

DOI: 10.1021/jp4070856

Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

In Situ IR Spectral Observation of NH₄H₂PO₄ Crystallization: Structural Identification of Nucleation and Crystal Growth

Congting Sun and Dongfeng Xue

pp 19146–19153

Publication Date (Web): August 20, 2013 (Article)

DOI: 10.1021/jp407947s



Section:

Crystallography and Liquid Crystals

Active Plasmonic Nanoantennas for Controlling Fluorescence Beams

Haibo Li, Shuping Xu, Yuejiao Gu, Hailong Wang, Renping Ma, John R. Lombardi, and Weiqing Xu

pp 19154–19159

Publication Date (Web): August 22, 2013 (Article)

DOI: 10.1021/jp408201z



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Physical Processes in Nanomaterials and Nanostructures

Regioselective Oxidation of Strained Graphene for Controllable Synthesis of Nanoribbons

Xin Tan and Peter Zapol

pp 19160–19166

Publication Date (Web): August 15, 2013 (Article)

DOI: 10.1021/jp402312k



Section:

Surface Chemistry and Colloids

Thermal-Induced Structural Evolution of Carbon-Encapsulated Iron Nanoparticles Generated by Two Different Methods

Noemí Aguiló-Aguayo, Zhenyu Liu, Enric Bertran, and Judith Yang

pp 19167–19174

Publication Date (Web): August 12, 2013 (Article)

DOI: 10.1021/jp4025552



Section:

Surface Chemistry and Colloids

Synthesis of High-Quality N-Acetyl-L-Cysteine-Capped CdTe Quantum Dots by Hydrothermal Route and the Characterization through MALDI-TOF Mass Spectrometry

Jiaotian Li, Tianming Yang, W. H. Chan, Martin M. F. Choi, and Dan Zhao

pp 19175–19181

Publication Date (Web): September 9, 2013 (Article)

DOI: 10.1021/jp402951c



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Femtosecond Pulse-Width Dependent Trapping and Directional Ejection Dynamics of Dielectric Nanoparticles

Wei-Yi Chiang, Anwar Usman, and Hiroshi Masuhara

pp 19182–19188

Publication Date (Web): August 16, 2013 (Article)

DOI: 10.1021/jp404372a



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

Spatially Sequential Growth of Various WS₂ Networked Nanostructures and Mechanisms

Mohammad Norouzi Banis, Xiangbo Meng, Yong Zhang, Mei Cai, Ruying Li, and Xueliang Sun

pp 19189–19194

Publication Date (Web): August 13, 2013 (Article)

DOI: 10.1021/jp404444p



Section:

Industrial Inorganic Chemicals

Controlled and Selective Area Growth of Monolayer Graphene on 4H-SiC Substrate by Electron-Beam-Assisted Rapid Heating

P. Dharmaraj, K. Jeganathan, V. Gokulakrishnan, P. Sundara Venkatesh, R. Parameshwari, V. Ramakrishnan, S. Balakumar, K. Asokan, and K. Ramamurthi

pp 19195–19202

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp404483y



Section:

Crystallography and Liquid Crystals

Equivalent Permittivity and Permeability and Multiple Fano Resonances for Nonlocal Metallic Nanowires

Y. Huang and L. Gao

pp 19203–19211

Publication Date (Web): August 20, 2013 (Article)

DOI: 10.1021/jp404490m



Section:

Optical, Electron, and Mass Spectroscopy and Other Related Properties

A Technique To Pretreat Graphite Which Allows the Rapid Dispersion of Defect-Free Graphene in Solvents at High Concentration

Sebastian Barwich, Umar Khan, and Jonathan N. Coleman

pp 19212–19218

Publication Date (Web): August 19, 2013 (Article)

DOI: 10.1021/jp4047006



Industrial Inorganic Chemicals

Carbon Nanodots-Catalyzed Chemiluminescence of Luminol: A Singlet Oxygen-Induced Mechanism

Dong Mei Wang, Ming Xuan Gao, Peng Fei Gao, Hui Yang, and Cheng Zhi Huang

pp 19219–19225

Publication Date (Web): August 21, 2013 (Article)

DOI: 10.1021/jp404973b



Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes

Diffusiophoresis of a Charged Sphere in a Necked Nanopore

Ting-Wen Lo, Chien Hsu, Kuan-Liang Liu, Jyh-Ping Hsu, and Shiojenn Tseng

pp 19226–19233

Publication Date (Web): September 4, 2013 (Article)

DOI: 10.1021/jp404975h



Surface Chemistry and Colloids

Unequal P Distribution in Nanowires and the Planar Layer during GaAsP Growth on GaAs {111}B by Metal–Organic Chemical Vapor Deposition

Wen Sun, Ya-Nan Guo, Hong-Yi Xu, Zhi-Ming Liao, Qiang Gao, Hark Hoe Tan, Chennupati Jagadish, and Jin Zou

pp 19234–19238

Publication Date (Web): August 23, 2013 (Article)

DOI: 10.1021/jp406294t



Section:

Electric Phenomena

Stability and Hydrogen Affinity of Graphite-Supported Wires of Cu, Ag, Au, Ni, Pd, and Pt

Germán J. Soldano, Paola Quaino, Elizabeth Santos, and Wolfgang Schmickler

pp 19239–19244

Publication Date (Web): August 26, 2013 (Article)

DOI: 10.1021/jp406361s



Section:

Surface Chemistry and Colloids

Additive-Free Assemblies of Ramified Single-Walled Carbon Nanotubes

Emeline Remy, Claire Hérolde, Fabrice Valsaque, Jean-François Marêché, Sébastien Fontana, Alexandre Desforges, Sébastien Cahen, Jaafar Ghanbaja, Jérôme Gleize, and Brigitte Vigolo

pp 19245–19252

Publication Date (Web): August 22, 2013 (Article)

DOI: 10.1021/jp406396y



Section:

Ceramics

Additions and Corrections

Correction to “On the Electrochemical Response of Porous Functionalized Graphene Electrodes”

Christian Punckt, Michael A. Pope, and Ilhan A. Aksay

pp 19253–19253

Publication Date (Web): September 9, 2013 (Addition/Correction)

DOI: 10.1021/jp408701v