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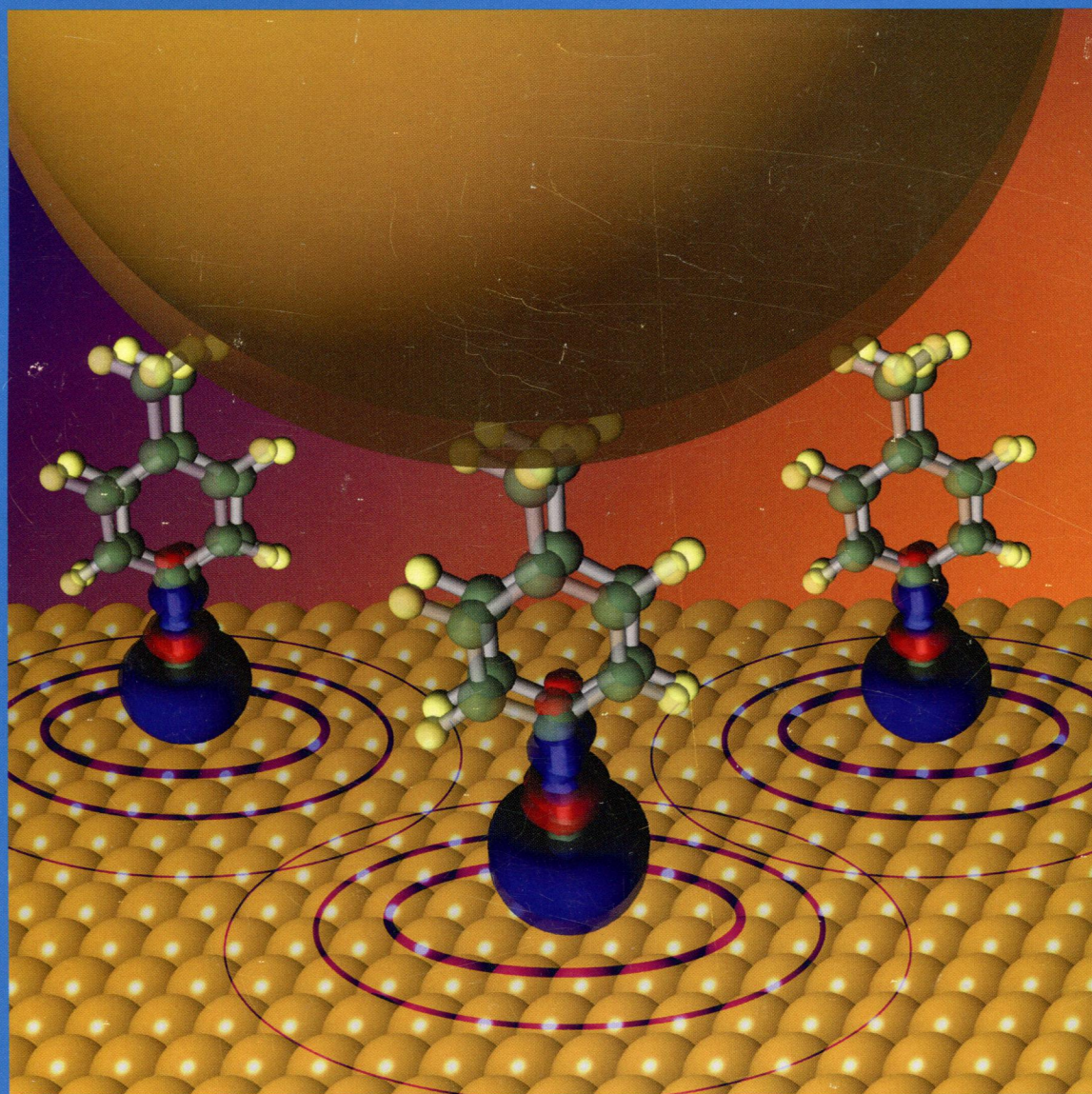
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Electron Donation
from Mechanically
Compressed Isocyanide
Molecules to the
Au(111) Substrate
(see page 21550)

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



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ON THE COVER: Electron donation from mechanically compressed isocyanide molecules to the Au(111) substrate. Orientational and electronic responses of molecular monolayers to optical near-fields and mechanical compression. The image shows isocyanide molecules on Au(111), which are sandwiched with an Au nanoparticle. The spatially confined optical fields exert a torque on the molecules in the nanogap. The mechanical compression of the gap distance not only disturbs the molecular alignments but also induces electron donation to Au(111). See page 21550.

Feature Article

21301

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Nanostructuring Materials for Solar-to-Hydrogen Conversion

Turgut M. Gür, Stacey F. Bent,* and Fritz B. Prinz

Articles

Energy Conversion and Storage; Energy and Charge Transport

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Energetic Performances of “ZIF-71–Aqueous Solution” Systems: A Perfect Shock-Absorber with Water

Guillaume Ortiz, Habiba Nouali, Claire Marichal, Gérald Chaplais,* and Joël Patarin*

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dx.doi.org/10.1021/jp5058786

Anisotropic Lattice Expansion of Structure H Clathrate Hydrates Induced by Help Guest: Experiments and Molecular Dynamics Simulations

Kotaro Murayama, Satoshi Takeya, Saman Alavi, and Ryo Ohmura*

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Shape-Dependent Charge Transfers in Crystalline ZnO Photocatalysts: Rods versus Plates

Hye Won Jeong, Seung-Yo Choi, Seong Hui Hong, Sang Kyoo Lim,* Dong Suk Han, Ahmed Abdel-Wahab, and Hyunwoong Park*

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dx.doi.org/10.1021/jp506111a

Vacancy Effects on Electric and Thermoelectric Properties of Zigzag Silicene Nanoribbons

Rui-Li An, Xue-Feng Wang,* P. Vasilopoulos, Yu-Shen Liu, An-Bang Chen, Yao-Jun Dong, and Ming-Xing Zhai

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[dx.doi.org/10.1021/jp506288w](https://doi.org/10.1021/jp506288w)**Earth-Abundant Metal Pyrites (FeS₂, CoS₂, NiS₂, and Their Alloys) for Highly Efficient Hydrogen Evolution and Polysulfide Reduction Electrocatalysis**

Matthew S. Faber, Mark A. Lukowski, Qi Ding, Nicholas S. Kaiser, and Song Jin*

21357 [dx.doi.org/10.1021/jp506856f](https://doi.org/10.1021/jp506856f)**Tunable Power Switching in Nonvolatile Flexible Memory Devices Based on Graphene Oxide Embedded with ZnO Nanorods**

Geetika Khurana, Pankaj Misra,* Nitu Kumar, and Ram S. Katiyar*

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[dx.doi.org/10.1021/jp5070648](https://doi.org/10.1021/jp5070648)**Magnetic Field Effects in Fluorescence of Exciplex and Fluorophore for the Weller Schemes I and II: Similarities and Differences**


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21377 [dx.doi.org/10.1021/jp507353g](https://doi.org/10.1021/jp507353g)**Charge Photogeneration Dynamics of Poly(3-hexylthiophene) Blend with Covalently-Linked Fullerene Derivative in Low Fraction**

Ning-Jiu Zhao, Zi-Hong Lin, Wei Zhang, Juan Liu, Yu-Wei Wang, Yu-Jun Qin, Xi-Cheng Ai, Zhi-Xin Guo, and Jian-Ping Zhang*

21385 [dx.doi.org/10.1021/jp507872d](https://doi.org/10.1021/jp507872d)**Elucidation of Aqueous Solvent-Mediated Hydrogen-Transfer Reactions by *ab Initio* Molecular Dynamics and Nudged Elastic-Band Studies of NaBH₄ Hydrolysis**

Ping Li, Graeme Henkelman, John A. Keith, and J. Karl Johnson*

21400 [dx.doi.org/10.1021/jp5082752](https://doi.org/10.1021/jp5082752)**Key Role of End-Capping Groups in Optoelectronic Properties of Poly-*p*-phenylene Cation Radicals**

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21420 [dx.doi.org/10.1021/jp507199z](https://doi.org/10.1021/jp507199z)**Molecular and Electronic Structure of Self-Assembled Monolayers Containing Ruthenium(II) Complexes on Gold Surfaces**


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21428 [dx.doi.org/10.1021/jp504695m](https://doi.org/10.1021/jp504695m)**Density Functional Investigation of the Adsorption of Isooctane, Ethanol, and Acetic Acid on a Water-Covered Fe(100) Surface**

Pedro O. Bedolla,* Gregor Feldbauer, Michael Wolloch, Christoph Gruber, Stefan J. Eder, Nicole Dörr, Peter Mohn, Josef Redinger, and Andrés Vernes

21438 [dx.doi.org/10.1021/jp505216v](https://doi.org/10.1021/jp505216v)**Theoretical Investigation of Small Transition-Metal Clusters Supported on the CeO₂(111) Surface**

Mauricio J. Piotrowski,* Polina Tereshchuk,* and Juarez L. F. Da Silva*

21447 [dx.doi.org/10.1021/jp505783y](https://doi.org/10.1021/jp505783y)**Generation of Reactive Oxygen Species, Electrons/Holes, and Photocatalytic Degradation of Rhodamine B by Photoexcited CdS and Ag₂S Micro-Nano Structures**

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[dx.doi.org/10.1021/jp505854t](https://doi.org/10.1021/jp505854t)**A Comparative Theoretical Study of Proton-Coupled Hole Transfer for H₂O and Small Organic Molecules (CH₃OH, HCOOH, H₂CO) on the Anatase TiO₂(101) Surface**

Yongfei Ji, Bing Wang, and Yi Luo*

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[dx.doi.org/10.1021/jp505971w](https://doi.org/10.1021/jp505971w)**Adsorption of CO Molecules on Si(001) at Room Temperature**

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21469 [dx.doi.org/10.1021/jp505978h](https://doi.org/10.1021/jp505978h)**Floating Patches of HCN at the Surface of Their Aqueous Solutions – Can They Make “HCN World” Plausible?**

Balázs Fábián, Milán Szőri,* and Pál Jedlovský*

21483 [dx.doi.org/10.1021/jp506158c](https://doi.org/10.1021/jp506158c)**Periodic DFT Study of Benzene Adsorption on Pd(100) and Pd(110) at Medium and Saturation Coverage**

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21500 [dx.doi.org/10.1021/jp5062489](https://doi.org/10.1021/jp5062489)**N₂ Selectivity of NO Reduction by NH₃ over MnO_x-CeO₂: Mechanism and Key Factors**

Shijian Yang,* Yong Liao, Shangchao Xiong, Feihong Qi, Hao Dang, Xin Xiao, and Junhua Li*

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[dx.doi.org/10.1021/jp506304d](https://doi.org/10.1021/jp506304d)**Reaction Mechanism and Regioselectivity of Methyl Oxirane on Si(111)-(7 × 7)**

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

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[dx.doi.org/10.1021/jp506444f](https://doi.org/10.1021/jp506444f)**Exploring the Surface Chemical Reactivity of Single Crystals of Binary and Ternary Bismuth Chalcogenides**

A. Politano,* M. Caputo, S. Nappini, F. Bondino, E. Magnano, Z. S. Aliev, M. B. Babanly, A. Goldoni, G. Chiarello, and E. V. Chulkov

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[dx.doi.org/10.1021/jp506544n](https://doi.org/10.1021/jp506544n)**Stability, Hydration, and Thermodynamic Properties of RNase A Confined in Surface-Functionalized SBA-15 Mesoporous Molecular Sieves**

Marie Kahse, Mayke Werner, Shuang Zhao, Martin Hartmann, Gerd Buntkowsky, and Roland Winter*

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[dx.doi.org/10.1021/jp5070215](https://doi.org/10.1021/jp5070215)**Graphene CVD: Interplay Between Growth and Etching on Morphology and Stacking by Hydrogen and Oxidizing Impurities**

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[dx.doi.org/10.1021/jp5071902](https://doi.org/10.1021/jp5071902)**Active Sites on Nanocrystalline Tin Dioxide Surface: Effect of Palladium and Ruthenium Oxides Clusters**

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Plasmonics, Optical Materials, and Hard Matter

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[dx.doi.org/10.1021/jp5036426](https://doi.org/10.1021/jp5036426)**Nanoscale Optical and Mechanical Manipulation of Molecular Alignment in Metal–Molecule–Metal Structures**

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[dx.doi.org/10.1021/jp506190h](https://doi.org/10.1021/jp506190h)**Tamm State-Coupled Emission: Effect of Probe Location and Emission Wavelength**

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Physical Processes in Nanomaterials and Nanostructures

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[dx.doi.org/10.1021/jp5025735](https://doi.org/10.1021/jp5025735)**In Situ Observation of Epitaxial Li–Si–Nanostructure Formation on Si(111)**

F. Grosse,* A. Proessdorf, M. Hanke, and O. Bierwagen

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[dx.doi.org/10.1021/jp5015252](https://doi.org/10.1021/jp5015252)**Tight-Binding Quantum Chemical Molecular Dynamics Simulations of Mechanisms of SiO₂ Etching Processes for CF₂ and CF₃ Radicals**

Hiroshi Ito, Takuya Kuwahara, Kentaro Kawaguchi, Yuji Higuchi, Nobuki Ozawa, Seiji Samukawa, and Momoji Kubo*

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[dx.doi.org/10.1021/jp5033195](https://doi.org/10.1021/jp5033195)**Facet Selectivity of Ligands on Silver Nanoplates: Molecular Mechanics Study**

Zhiye Tang, Qiao Zhang, Yadong Yin, and Chia-en A. Chang*

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Controlling the Electrical Response of Carbon Nanotubes Deposited on Diamond through the Application of Electric Fields
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Cadmium Vacancy Minority Defects as Luminescence Centers in Size and Strain Dependent Photoluminescence Shifts in CdS Nanotubes

Arthur Varghese, Prasenjit Ghosh,* and Shouvik Datta

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Behavior of As(V) with ZVI–H₂O System and the Reduction to As(0)

Priyanka Mondal, Subhamoy Bhowmick, Nora Jullok, Wen Yuan Ye, Wouter Van Renterghem, Sven Van den Berghe, and Bart Van der Bruggen*

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Magnetic Interactions in Spin-Labeled Au Nanoparticles

V. Lloveras, E. Badetti, V. Chechik,* and J. Vidal-Gancedo*

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Inhibition of Amyloid Fibril Growth by Nanoparticle Coated with Histidine-Based Polymer

Sharbari Palmal, Nihar R. Jana,* and Nikhil R. Jana*

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Probing the Structure of NaYF₄ Nanocrystals using Synchrotron-Based Energy-Dependent X-ray Photoelectron Spectroscopy

Jothirmayanantham Pichaandi, Gautom Kumar Das, Noah J. J. Johnson, Tom Regier, and Frank C. J. M. van Veggel*

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The Concept of Localized Atomic Mobility: Unraveling Properties of Nanoparticles

Renato G. Capelo, Linn Leppert, and Rodrigo Q. Albuquerque*

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Structural versus Electrical Functionalization of Oligo(phenylene ethynylene) Diamine Molecular Junctions

M. Teresa González,* Xiaotao Zhao, David Zsolt Manrique, Delia Miguel, Edmund Leary, Murat Gulcur, Andrei S. Batsanov, Gabino Rubio-Bollinger, Colin J. Lambert, Martin R. Bryce, and Nicolás Agrait

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Proton Transport through Robust CPO-27-type Metal Organic Frameworks

Cecilia Solís, Daniel Palaci, Francesc X. Llabrés i Xamena,* and José M. Serra*

21671 [dx.doi.org/10.1021/jp506361b](https://doi.org/10.1021/jp506361b)**Synthesis and Photophysics of Quaterylene Molecules in Single-Walled Carbon Nanotubes: Excitation Energy Transfer between a Nanoscale Cylinder and Encapsulated Molecules**

Takeshi Koyama,* Takuya Tsunekawa, Takeshi Saito, Koji Asaka, Yahachi Saito, Hideo Kishida, and Arao Nakamura

21682 [dx.doi.org/10.1021/jp506536h](https://doi.org/10.1021/jp506536h)**Ultra Long-Lived Radiative Trap States in CdSe Quantum Dots**


Mohamed Abdellah, Khadga J. Karki,* Nils Lenngren, Kaibo Zheng, Torbjörn Pascher, Arkady Yartsev, and Tõnu Pullerits*

21687 [dx.doi.org/10.1021/jp506689n](https://doi.org/10.1021/jp506689n)**Charge Transport through Carbon Nanomembranes**

Paul Penner, Xianghui Zhang,* Emanuel Marschewski, Florian Behler, Polina Angelova, André Beyer, Jens Christoffers, and Armin Götzhäuser

21695 [dx.doi.org/10.1021/jp5068582](https://doi.org/10.1021/jp5068582)**Observation of Ferroelectricity and Structure-Dependent Magnetic Behavior in Novel One-Dimensional Motifs of Pure, Crystalline Yttrium Manganese Oxides**

Jonathan M. Patete, Jinkyu Han, Amanda L. Tiano, Haiqing Liu, Myung-Geun Han, J. W. Simonson, Yuanyuan Li, Alexander C. Santulli, M. C. Aronson, Anatoly I. Frenkel, Yimei Zhu, and Stanislaus S. Wong*

21706 [dx.doi.org/10.1021/jp507266t](https://doi.org/10.1021/jp507266t)**Glass, Gel, and Liquid Crystals: Arrested States of Graphene Oxide Aqueous Dispersions**

Bharathi Konkena and Sukumaran Vasudevan*

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[dx.doi.org/10.1021/jp507382z](https://doi.org/10.1021/jp507382z)**Element-Specific Analysis of the Growth Mechanism, Local Structure, and Electronic Properties of Pt Clusters Formed on Ag Nanoparticle Surfaces**

Paul N. Duchesne and Peng Zhang*

21722 [dx.doi.org/10.1021/jp508124b](https://doi.org/10.1021/jp508124b)**Ag₁₁(SG)₇: A New Cluster Identified by Mass Spectrometry and Optical Spectroscopy**

Ananya Baksi, M. S. Bootharaju, Xi Chen, H. Häkkinen, and T. Pradeep*

21730 [dx.doi.org/10.1021/jp508419p](https://doi.org/10.1021/jp508419p)**Impact of the Selenolate Ligand on the Bonding Behavior of Au₂₅ Nanoclusters**


Daniel M. Chevrier, Xiangming Meng, Qing Tang, De-en Jiang, Manzhou Zhu, Amare Chatt, and Peng Zhang*

Comments

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[dx.doi.org/10.1021/jp5054524](https://doi.org/10.1021/jp5054524)**Comment on "Rapid and Efficient Prediction of Optical Extinction Coefficients for Gold Nanospheres and Gold Nanorods"**

Maxim A. Yurkin*

 Supporting Information available via online article