

J 80/pc 2

JUNE 12, 2014

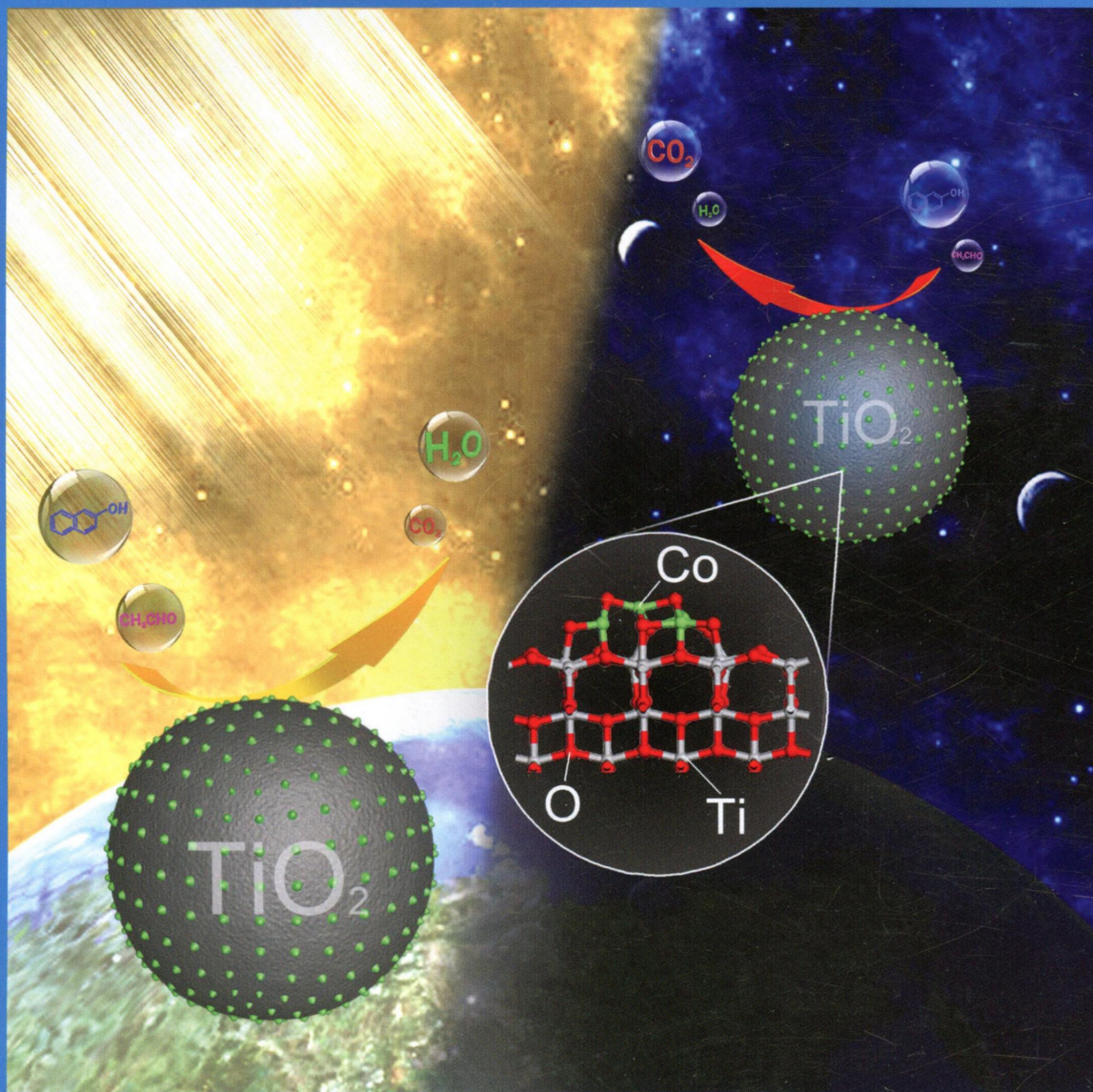
VOLUME 118

NUMBER 23

pubs.acs.org/JPCC

THE JOURNAL OF PHYSICAL CHEMISTRY

C



Environmental
Purification by
Cobalt Oxide Cluster
Surface-Modified TiO_2
Night and Day
(see page 12077)

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



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org


ON THE COVER: Environmental purification by cobalt oxide cluster surface-modified TiO₂ night and day. The development of environmental catalysts is an urgent subject to be tackled by scientists and engineers all over the world due to the borderless nature of the environmental pollution. A combination of experiments and first-principles density functional theory simulations shows that Co₂O₃/TiO₂ can be a prototype of the solar environmental catalyst with high levels of photo- (UV and visible) and thermocatalytic activities. See page 12077.


Feature Article


12077 [dx.doi.org/10.1021/jp412312m](https://doi.org/10.1021/jp412312m)
Molecular-Scale Transition Metal Oxide Nanocluster Surface-Modified Titanium Dioxide as Solar-Activated Environmental Catalysts
Hiroaki Tada,* Qiliang Jin, Anna Iwaszuk, and Michael Nolan*

Articles

Energy Conversion and Storage; Energy and Charge Transport






12087  [dx.doi.org/10.1021/jp411265b](https://doi.org/10.1021/jp411265b)
Fully Reversible De/hydriding of Mg Base Solid Solutions with Reduced Reaction Enthalpy and Enhanced Kinetics
Hui Wang, Haichang Zhong, Liuzhang Ouyang, Jiangwen Liu, Dalin Sun, Qingan Zhang, and Min Zhu*

12097  [dx.doi.org/10.1021/jp5012507](https://doi.org/10.1021/jp5012507)
First-Principles Analysis of Potential-Dependent Proton Coupled Electron Transfer between Polypyridyl–Ruthenium Complexes and Oxygen-Modified Graphene Electrodes
Yu Cai and Matthew Neurock*

12106  [dx.doi.org/10.1021/jp5013208](https://doi.org/10.1021/jp5013208)
Experimental and Theoretical Analysis of Products and Reaction Intermediates of Lithium–Sulfur Batteries
Natalia A. Cañas, David N. Fronczek, Norbert Wagner,* Arnulf Latz, and K. Andreas Friedrich

12115  [dx.doi.org/10.1021/jp501954m](https://doi.org/10.1021/jp501954m)
Structures and Electronic Properties of Heavier Congeners of Disk-Like Molecules: (Si, Ge) Sulfollower and (Si, Ge) Olympicene
Tarun K. Mandal,* Deepthi Jose, A. Nijamudheen, and Ayan Datta*

- 12121  [dx.doi.org/10.1021/jp502122d](https://doi.org/10.1021/jp502122d)
Two Thin Film Polymorphs of the Singlet Fission Compound 1,3-Diphenylisobenzofuran
Joseph L. Ryerson, Joel N. Schrauben, Andrew J. Ferguson, Subash Chandra Sahoo, Panče Naumov, Zdeněk Havlas, Josef Michl, Arthur J. Nozik, and Justin C. Johnson*
- 12133  [dx.doi.org/10.1021/jp5023604](https://doi.org/10.1021/jp5023604)
Electron–Hole Pair Generation of the Visible-Light Plasmonic Photocatalyst Ag@AgCl: Enhanced Optical Transitions Involving Midgap Defect States of AgCl
Xiangchao Ma, Ying Dai,* Lin Yu, Zaizhu Lou, Baibiao Huang, and Myung-Hwan Whangbo
- 12141  [dx.doi.org/10.1021/jp502788j](https://doi.org/10.1021/jp502788j)
Synthesis, Crystal Structure, Thermal Decomposition, and ¹¹B MAS NMR Characterization of Mg(BH₄)₂(NH₃BH₃)₂
Lars H. Jepsen, Voraksmy Ban, Kasper T. Møller, Young-Su Lee, Young Whan Cho, Flemming Besenbacher, Yaroslav Filinchuk, Jørgen Skibsted, and Torben R. Jensen*
- 12154 [dx.doi.org/10.1021/jp5030075](https://doi.org/10.1021/jp5030075)
Remarkable Fluorescence Enhancement versus Complex Formation of Cationic Porphyrins on the Surface of ZnO Nanoparticles
Shawkat M. B. Aly, Mohamed Eita, Jafar I. Khan, Erkki Alarousu, and Omar F. Mohammed*
- 12162  [dx.doi.org/10.1021/jp503226r](https://doi.org/10.1021/jp503226r)
Mechanism and Kinetic Study of the Electrochemical Charge and Discharge of La₂MgNi₉ by in Situ Powder Neutron Diffraction
Michel Latroche,* Fermin Cuevas, Wei-Kang Hu, Denis Sheptyakov, Roman V. Denys, and Volodymyr A. Yartys
- 12170 [dx.doi.org/10.1021/jp503298e](https://doi.org/10.1021/jp503298e)
Hopping Conductivity and Polarization Effects in a Fullerene Derivative Salt
Roberto Macovez,* Manesh Zachariah, Michela Romanini, Panagiota Zygouri, Dimitrios Gournis, and Josep Lluís Tamarit
- 12176 [dx.doi.org/10.1021/jp504479c](https://doi.org/10.1021/jp504479c)
Cation Role in Structural and Electronic Properties of 3D Organic–Inorganic Halide Perovskites: A DFT Analysis
Giacomo Giorgi,* Jun-Ichi Fujisawa, Hiroshi Segawa, and Koichi Yamashita*
- Surfaces, Interfaces, Porous Materials, and Catalysis**
- 12184  [dx.doi.org/10.1021/jp409718x](https://doi.org/10.1021/jp409718x)
Infrared Spectroscopy of Ammonia on Iron: Thermal Stability and the Influence of Potassium
P. Iyngaran, D. C. Madden, D. A. King, and S. J. Jenkins*
- 12195  [dx.doi.org/10.1021/jp502383u](https://doi.org/10.1021/jp502383u)
Interaction of Polyethylenimine with Model Cell Membranes Studied by Linear and Nonlinear Spectroscopic Techniques
Chi Zhang, Fu-Gen Wu, Peipei Hu, and Zhan Chen*

- 12206  [dx.doi.org/10.1021/jp4120964](https://doi.org/10.1021/jp4120964)
Evaluating the Mechanism of Visible Light Activity for N,F-TiO₂ Using Photoelectrochemistry
Jeremy W.J. Hamilton,* J. Anthony Byrne, Patrick S.M. Dunlop, Dionysios D. Dionysiou, Miguel Pelaez, Kevin O'Shea, Damian Synnott, and Suresh C. Pillai
- 12216 [dx.doi.org/10.1021/jp503745c](https://doi.org/10.1021/jp503745c)
Single Pd Atom Embedded in CeO₂(111) for NO Reduction with CO: A First-Principles Study
Wu-Chen Ding, Xiang-Kui Gu, Hai-Yan Su, and Wei-Xue Li*
- 12224 [dx.doi.org/10.1021/jp500287u](https://doi.org/10.1021/jp500287u)
Influence of Surface Symmetry on the Onset of Nitrogen Eley-Rideal Recombination on Tungsten
E. Quintas-Sánchez, P. Larrégaray,* and C. Crespos
- 12230  [dx.doi.org/10.1021/jp500313j](https://doi.org/10.1021/jp500313j)
CO₂ Adsorption in Fe₂(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations
Joshua Borycz, Li-Chiang Lin, Eric D. Bloch, Jihan Kim, Allison L. Dzubak, Rémi Maurice, David Semrouni, Kyuho Lee, Berend Smit,* and Laura Gagliardi*
- 12241  [dx.doi.org/10.1021/jp501030h](https://doi.org/10.1021/jp501030h)
Oligo(*p*-phenyleneethynylene)-Derived Porous Luminescent Nanoscale Coordination Polymer of Gd^{III}: Bimodal Imaging and Nitroaromatic Sensing
Venkata M. Suresh, Snehajyoti Chatterjee, Rahul Modak, Vivek Tiwari, Anant B. Patel, Tapas K. Kundu, and Tapas Kumar Maji*
- 12250 [dx.doi.org/10.1021/jp501326c](https://doi.org/10.1021/jp501326c)
Size-Controlled Pd Nanoparticles in 2-Butyne-1,4-diol Hydrogenation: Support Effect and Kinetics Study
Charline Berguerand, Igor Yuranov, Fernando Cárdenas-Lizana, Tatiana Yuranova, and Lioubov Kiwi-Minsker*
- 12260  [dx.doi.org/10.1021/jp501584f](https://doi.org/10.1021/jp501584f)
Ensemble Effect Evidenced by CO Adsorption on the 3-Fold PdGa Surfaces
Jan Prinzh, Roberto Gaspari, Quirin S. Stöckl, Peter Gille, Marc Armbrüster, Harald Brune, Oliver Gröning, Carlo A. Pignedoli, Daniele Passerone, and Roland Widmer*
- 12266  [dx.doi.org/10.1021/jp501928k](https://doi.org/10.1021/jp501928k)
2,6-Di-*tert*-butylpyridine Sorption Approach to Quantify the External Acidity in Hierarchical Zeolites
Kinga Góra-Marek,* Karolina Tarach, and Minkee Choi
- 12275 [dx.doi.org/10.1021/jp502179n](https://doi.org/10.1021/jp502179n)
Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory
Chiara Ricca, Frédéric Labat,* Nino Russo, Carlo Adamo, and Emilia Sicilia*

12285 [dx.doi.org/10.1021/jp5025075](https://doi.org/10.1021/jp5025075)

Semihydrogenation of Acetylene on the (010) Surface of GaPd₂: Ga Enrichment Improves Selectivity

M. Krajčí* and J. Hafner

12302 [dx.doi.org/10.1021/jp5025137](https://doi.org/10.1021/jp5025137)

Thermal, Oxidative and CO₂ Induced Degradation of Primary Amines Used for CO₂ Capture: Effect of Alkyl Linker on Stability

Stephanie A. Didas, Rongshun Zhu, Nicholas A. Brunelli, David S. Sholl, and Christopher W. Jones*

12312 [dx.doi.org/10.1021/jp5025763](https://doi.org/10.1021/jp5025763)

Two-Electron Transfer Reactions in Electrochemistry for Solution-Soluble and Surface-Confined Molecules: A Common Approach

Manuela Lopez-Tenes, Joaquin Gonzalez, and Angela Molina*

12325 [dx.doi.org/10.1021/jp502596n](https://doi.org/10.1021/jp502596n)

Effect of O₃ on Growth of Pt by Atomic Layer Deposition

Han-Bo-Ram Lee, Katie L. Pickrahn, and Stacey F. Bent*

12333 [dx.doi.org/10.1021/jp502729u](https://doi.org/10.1021/jp502729u)

Observation of Distinct Bulk and Surface Chemical Environments in a Topological Insulator under Magnetic Doping

Ivana Vobornik,* Giancarlo Panaccione,* Jun Fujii, Zhi-Huai Zhu, Francesco Offi, Benjamin R. Salles, Francesco Borgatti, Piero Torelli, Jean Pascal Rueff, Denis Ceolin, Alberto Artioli, Manju Unnikrishnan, Giorgio Levy, Massimiliano Marangolo, Mamhoud Eddrief, Damjan Krizmancic, Huiwen Ji, Andrea Damascelli, Gerrit van der Laan, Russell G. Egdell, and Robert J. Cava

12340 [dx.doi.org/10.1021/jp502748a](https://doi.org/10.1021/jp502748a)

Effect of a Gold Cover Layer on the Encapsulation of Rhodium by Titanium Oxides on Titanium Dioxide(110)

László Óvári,* András Berkó, Richárd Gubó, Árpád Rácz, and Zoltán Kónya

12353 [dx.doi.org/10.1021/jp502893x](https://doi.org/10.1021/jp502893x)

Adsorption Properties of Two-Dimensional NaCl: A Density Functional Theory Study of the Interaction of Co, Ag, and Au Atoms with NaCl/Au(111) Ultrathin Films

Hsin-Yi Tiffany Chen, Livia Giordano, and Gianfranco Pacchioni*

12364 [dx.doi.org/10.1021/jp503056u](https://doi.org/10.1021/jp503056u)

Following Molecules through Reactive Networks: Surface Catalyzed Decomposition of Methanol on Pd(111), Pt(111), and Ni(111)

Zeb C. Kramer, Xiang-Kui Gu, Dingyu D. Y. Zhou, Wei-Xue Li,* and Rex T. Skodje*

12384 [dx.doi.org/10.1021/jp503292r](https://doi.org/10.1021/jp503292r)

Spectroscopic Investigation of the Selective Interaction of Mercuric and Cupric Ions with a Porphyrin Active Layer

Simona Bettini, Rosanna Pagano, Ludovico Valli, and Gabriele Giancane*

12391  [dx.doi.org/10.1021/jp5034855](https://doi.org/10.1021/jp5034855)

Surface Chemistry of CO on Ru(0001) under the Confinement of Graphene Cover
Li Jin, Qiang Fu,* Aiyi Dong, Yanxiao Ning, Zhoujun Wang, Hendrik Bluhm, and Xinhe Bao

12399  [dx.doi.org/10.1021/jp503497f](https://doi.org/10.1021/jp503497f)

Patterning Superhydrophobic Surfaces To Realize Anisotropic Wettability and To Transport Micro-Liter-Sized Droplets to Any Type of Surface
Chih-Feng Wang* and Tse-Wei Hsueh

12405 [dx.doi.org/10.1021/jp504374z](https://doi.org/10.1021/jp504374z)

Density Profiles of Liquid/Vapor Interfaces Away from Their Critical Points
Wei Bu, Doseok Kim, and David Vaknin*


Plasmonics, Optical Materials, and Hard Matter

12410 [dx.doi.org/10.1021/jp4112926](https://doi.org/10.1021/jp4112926)

Lattice Dynamic Behavior of Orthoferrosilite (FeSiO₃) toward Phase Transition under Compression
Jennifer Kung* and Baosheng Li

12420  [dx.doi.org/10.1021/jp412065p](https://doi.org/10.1021/jp412065p)

Pressure-Induced Diversity of π -Stacking Motifs and Amorphous Polymerization in Pyrrole
Wenbo Li, Defang Duan, Xiaoli Huang, Xilian Jin, Xue Yang, Shourui Li, Shuqing Jiang, Yanping Huang, Fangfei Li, Qiliang Cui, Qiang Zhou, Bingbing Liu, and Tian Cui*

12428  [dx.doi.org/10.1021/jp5002379](https://doi.org/10.1021/jp5002379)

Interplay between Crystal Structure and Photoluminescence Properties of β -Ca₃SiO₄Cl₂:Eu²⁺
Tae-Gon Kim,* Taehyung Kim, Jaegyem Kim, Seung-Joo Kim,* and Seoung-Jae Im

12436  [dx.doi.org/10.1021/jp5003758](https://doi.org/10.1021/jp5003758)


Formation of Photoluminescent Lead Bromide Nanoparticles on Aluminoborosilicate Glass
Andreia Ruivo, Suzana M. Andrade, João Rocha, César A. T. Laia,* and Fernando Pina

12443  [dx.doi.org/10.1021/jp500484a](https://doi.org/10.1021/jp500484a)

Electronic Structures of Platinum(II) Complexes with 2-Arylpyridine and 1,3-Diketonate Ligands: A Relativistic Density Functional Study on Photoexcitation and Phosphorescent Properties
Mie Tanaka and Hirotohi Mori*

12450  [dx.doi.org/10.1021/jp5016565](https://doi.org/10.1021/jp5016565)

Optical Properties of Silver Nanoshells from Time-Dependent Density Functional Theory Calculations
Giovanni Barcaro, Luca Sementa, Alessandro Fortunelli,* and Mauro Stener*

12459  [dx.doi.org/10.1021/jp501884s](https://doi.org/10.1021/jp501884s)
Edge-Gold-Coated Silver Nanoprisms: Enhanced Stability and Applications in Organic Photovoltaics and Chemical Sensing
Mohammad M. Shahjamali, Michael Salvador, Michel Bosman, David S. Ginger,* and Can Xue*

12469  [dx.doi.org/10.1021/jp502318s](https://doi.org/10.1021/jp502318s)
Analysis of the Resonant Raman Spectra of Viologens and of Their Radical Cations Using Range-Separated Hybrid Density Functionals
Julia Romanova, Vincent Liégeois, and Benoit Champagne*

12485 [dx.doi.org/10.1021/jp502550z](https://doi.org/10.1021/jp502550z)
Nanoscale Structure of Cement: Viewpoint of Rigidity Theory
Mathieu Bauchy,* Mohammad Javad Abdolhosseini Qomi, Christophe Bichara, Franz-Joseph Ulm, and Roland J.-M. Pellenq


12494 [dx.doi.org/10.1021/jp502571c](https://doi.org/10.1021/jp502571c)
Color-Tunable Phosphor of Eu^{2+} and Mn^{2+} Codoped $\text{Ca}_2\text{Sr}(\text{PO}_4)_2$ for UV Light-Emitting Diodes
Yan Chen, Ye Li, Jing Wang,* Mingmei Wu,* and Chengxin Wang

12500 [dx.doi.org/10.1021/jp503202f](https://doi.org/10.1021/jp503202f)
Improved Performance of Solution-Phase Surface-Enhanced Raman Scattering at Ag/CuO Nanocomposite Surfaces
Shuchen Hsieh,* Pei-Ying Lin, and Ling-Ya Chu

12506  [dx.doi.org/10.1021/jp503323u](https://doi.org/10.1021/jp503323u)
Aluminum and Indium Plasmonic Nanoantennas in the Ultraviolet
Michael B. Ross and George C. Schatz*

Physical Processes in Nanomaterials and Nanostructures

12515 [dx.doi.org/10.1021/jp411887s](https://doi.org/10.1021/jp411887s)
Enhanced Thermal Sensitivity of Silicon Nanoparticles Embedded in (Nano-Ag)/SiN_x for Luminescent Thermometry
Yury V. Ryabchikov, Vladimir Lysenko, and Tetyana Nychporuk*

12520  [dx.doi.org/10.1021/jp500499d](https://doi.org/10.1021/jp500499d)
Study on the Absorption Coefficient of Reduced Graphene Oxide Dispersion
Rui Su, Shao Fen Lin, Dan Qing Chen, and Guo Hua Chen*

12526 [dx.doi.org/10.1021/jp501897a](https://doi.org/10.1021/jp501897a)
Size Dependence of Compressive Strain in Graphene Flakes Directly Grown on SiO₂/Si Substrate
Yuqing Song, Jinyang Liu, Lin Quan, Nan Pan, Hong Zhu, and Xiaoping Wang*

12532 [dx.doi.org/10.1021/jp502215m](https://doi.org/10.1021/jp502215m)

Effect of Substrate Chemistry on the Bottom-Up Fabrication of Graphene Nanoribbons: Combined Core-Level Spectroscopy and STM Study

Konstantin A. Simonov,* Nikolay A. Vinogradov, Alexander S. Vinogradov, Alexander V. Generalov, Elena M. Zagrebina, Nils Mårtensson, Attilio A. Cafolla, Tomas Carpy, John P. Cunniffe, and Alexei B. Preobrajenski*

12541 [dx.doi.org/10.1021/jp502564e](https://doi.org/10.1021/jp502564e)

Thermal Conduction Across Graphene Cross-Linkers

Xiangjun Liu, Gang Zhang,* and Yong-Wei Zhang

12548 [dx.doi.org/10.1021/jp502565x](https://doi.org/10.1021/jp502565x)

Spatial Variation of Molecular Dynamics in the Nanoconfined Glass-Former Methanol

Andriy V. Kityk, Patrick Huber,* Rolf Pelster, and Klaus Knorr

12555 [dx.doi.org/10.1021/jp5029905](https://doi.org/10.1021/jp5029905)

Thermodynamic Stability of [60]Fullerene and γ -Cyclodextrin Complex in Aqueous Solution: Free Energy Simulation

Shunsuke Mieda, Atsushi Ikeda, Yasushi Shigeri, and Wataru Shinoda*

12562  [dx.doi.org/10.1021/jp503241p](https://doi.org/10.1021/jp503241p)

Unveiling the Underlying Mechanism for Compression and Decompression Strokes of a Molecular Engine

Peng Liu, Christophe Chipot, Wensheng Cai,* and Xueguang Shao*

12568  [dx.doi.org/10.1021/jp5038624](https://doi.org/10.1021/jp5038624)

Photoinduced Separation of Strongly Interacting 2-D Layered TiS₂ Nanodiscs in Solution

Daniel Rossi, Jae Hyo Han, Dongwon Yoo, Yitong Dong, Yerok Park, Jinwoo Cheon,* and Dong Hee Son*

Additions and Corrections

12574 [dx.doi.org/10.1021/jp504556j](https://doi.org/10.1021/jp504556j)

Correction to Plasmon Mediated Multiphoton Photoemission Microscopy of Au Nanoholes and Nanohole Dimers

Thomas A. Baker, Andrej Grubisic, and David J. Nesbitt*

12575 [dx.doi.org/10.1021/jp504875z](https://doi.org/10.1021/jp504875z)

Correction to "Structure Analysis of Al-Modified TiO₂ Nanocatalyst Supports"

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

12576 [dx.doi.org/10.1021/jp505195m](https://doi.org/10.1021/jp505195m)

Correction to "Anomalous Strong Electric Near-Field Enhancements at Defect Sites on Au Nanoshells Observed by Ultrafast Scanning Photoemission Imaging Microscopy"

Andrej Grubisic, Shaunak Mukherjee, Naomi Halas,* and David J. Nesbitt*