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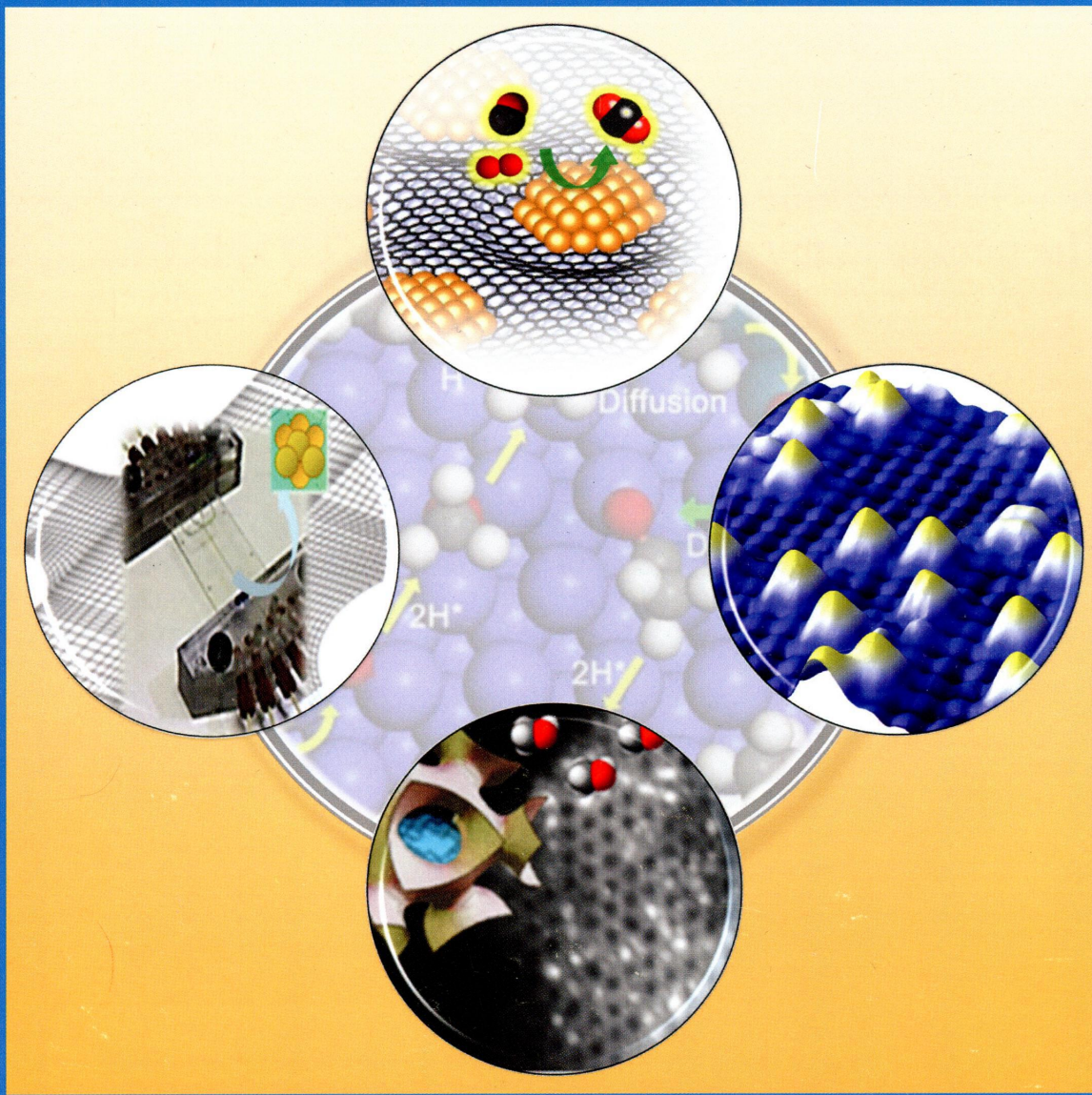
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THE JOURNAL OF PHYSICAL CHEMISTRY

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Synthesis,
Characterization, and
Computation—Working
Together
(see page 20043)



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

ON THE COVER: Synthesis, characterization, and computation—working together. Top: Catalysis by arrays of metal nanoclusters that are formed on corrugated thin film surfaces. Right: Atomically resolved scanning tunneling microscopy image of single gold atoms supported on a model catalyst. The atoms are thermally stable and stay dispersed up to temperatures of 700 K. Bottom: This image shows pore-confined metal nanoparticles on CuZnO/SiO₂ methanol synthesis catalysts. Reprinted with permission from: Prieto, G.; Shakeri, M.; de Jong, K.P.; de Jongh, P.E. Quantitative Relationship between Support Porosity and the Stability of Pore-Confined Metal Nanoparticles Studied on CuZnO/SiO₂ Methanol Synthesis Catalysts. *ACS Nano* **2014**, *8*, 2522–2531. Left: Geometric optimization of liquid–liquid slug flow in a flow-focusing millifluidic device for synthesis of nanomaterials. Adapted with permission from Elsevier: Li, Y.; Yamane, D. G.; Li, S.; Biswas, S.; Reddy, R. K.; Goettert, J. S.; Nandakumar, K.; Kumar, C. S. S. R. Geometric Optimization of Liquid–Liquid Slug Flow in a Flow-Focusing Millifluidic Device for Synthesis of Nanomaterials. *Chem. Eng. J.* **2013**, *217*, 447–459. Center: Computationally derived reaction mechanism for the conversion of syngas to ethanol on a cobalt–palladium nanocluster catalyst. Higher alcohols are formed only when short alkane fragments diffuse from highly active cobalt sites to Co–Pd interface sites capable of catalyzing CO insertion reactions. See page 20043.

Feature Article

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Synthesis, Characterization, and Computation of Catalysts at the Center for Atomic-Level Catalyst Design

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Boundary and Symmetry Determined Exciton Distribution in Two Dimensional Silicon Nanosheets

Qi Wu, Xiao-Hui Wang, T.A. Niehaus, and Rui-Qin Zhang*

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dx.doi.org/10.1021/jp503366m

Efficiency-Limiting Processes in Low-Bandgap Polymer:Perylene Diimide Photovoltaic Blends

Dominik W. Gehrig, Steffen Roland, Ian A. Howard, Valentin Kamm, Hannah Mangold, Dieter Neher, and Frédéric Laquai*

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dx.doi.org/10.1021/jp504055j

Electrochemical Properties of Electrodeposited Sn Anodes for Na-Ion Batteries

Do-Hwan Nam, Kyung-Sik Hong, Sung-Jin Lim, Tae-Hee Kim, and Hyuk-Sang Kwon*

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Wei-Chih Chen and Ito Chao*

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Effect of Molecular Nitrogen on Multiple Hydrogen Occupancy in Clathrate Hydrates

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Vishal Govind Rao, Bharat Dhital, Yufan He, and H. Peter Lu*

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Electronic Structure and Photoelectrochemical Properties of an Ir-Doped $SrTiO_3$ Photocatalyst

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La_2O_3 Doped Carbonaceous Microspheres: A Novel Bifunctional Electrocatalyst for Oxygen Reduction and Evolution Reactions with Ultrahigh Mass Activity

Xiaoxue Zhang, Qingqing Xiao, Yuxia Zhang, Xiong Jiang, Zhiyu Yang, Yifei Xue, Yi-Ming Yan,* and Kening Sun


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IR Selective Irradiations of Amorphous Solid Water Dangling Modes: Irradiation vs Annealing Effects

J. A. Noble, C. Martin, H. J. Fraser, P. Roubin, and S. Coussan*

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In Situ Spectroscopic Evidence for Ordered Core–Ultrathin Shell Pt₄Co₃ Nanoparticles with Enhanced Activity and Stability as Oxygen Reduction Electrocatalysts

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Microstructures of the Porphyrin/Viologen Monolayer on the Clay Surface: Segregation or Integration?

Saki Konno, Takuya Fujimura, Yuta Otani, Tetsuya Shimada, Haruo Inoue, and Shinsuke Takagi*

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Nature of Tunable Optical Reflectivity of Rocksalt Hafnium Nitride Films

Chaoquan Hu, Zhiqing Gu, Jianbo Wang, Kan Zhang, Xiaobo Zhang, Mingming Li, Sam Zhang, Xiaofeng Fan,* and Weitao Zheng*

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Micro–Nanosized Nontraditional Evaporated Structures Based on Closely Packed Monolayer Binary Colloidal Crystals and Their Fine Structure Enhanced Properties

Junfeng Zheng, Zhigao Dai, Fei Mei, Xiangheng Xiao,* Lei Liao, Wei Wu, Xinyue Zhao, Jianjian Ying, Feng Ren, and Changzhong Jiang*

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Competition of Chiroptical Effect Caused by Nanostructure and Chiral Molecules

Tong Wu, Jun Ren, Rongyao Wang, and Xiangdong Zhang*

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Phosphorescent Sensor Based on Iridium Complex/Poly(vinylcarbazole) Orderly Assembled with Layered Double Hydroxide Nanosheets: Two-Dimensional Förster Resonance Energy Transfer and Reversible Luminescence Response for VOCs

Yumei Qin, Jun Lu,* Shuangde Li, Zhen Li, and Shufang Zheng

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Hao Chen, Abdul M. Bhuiya, Runyu Liu, Daniel M. Wasserman, and Kimani C. Toussaint Jr.*

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Selectively Investigating Molecular Configuration Effect on Blue Electrophosphorescent Host Performance through a Series of Hydrocarbon Oligomers

Zhen Zhang, Zhensong Zhang, Dongxue Ding, Ying Wei, Hui Xu,* Jilin Jia, Yi Zhao,* Kai Pan, and Wei Huang*

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Analysis of Trap-State Dynamics of Single CdSe/ZnS Quantum Dots on a TiO_2 Substrate with Different Nb Concentrations

Yuki Nagao, Hideki Fujiwara,* and Keiji Sasaki*

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Božidar Nikolić,* Ivanka Milošević, and Milan Damjanović

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Size Dependence of Temperature-Related Optical Properties of PbS and PbS/CdS Core/Shell Quantum Dots

Haiguang Zhao, Hongyan Liang, François Vidal, Federico Rosei, Alberto Vomiero, and Dongling Ma*

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Numerical Simulations of Stick Percolation: Application to the Study of Structured Magnetorheological Elastomers

J. L. Mietta, R. M. Negri, and P. I. Tamborenea*

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Predictions of the Spin Configuration in Mn_{12} Molecular Magnets Made Accurate with the Help of Hubbard U on the Ligand Atoms

Shruba Gangopadhyay, Artëm E. Masunov,* and Svetlana Kilina

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Position-Controlled Hydrothermal Growth of Periodic Individual ZnO Nanorod Arrays on Indium Tin Oxide Substrate

Tonghui Yang, Ke Cheng, Gang Cheng, Binbin Hu, Shujie Wang, and Zuliang Du*

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Anisotropic Electrical Properties from Vapor–Solid–Solid Grown Bi₂Se₃ Nanoribbons and Nanowires
Yichao Zou, Zhi-Gang Chen,* Yang Huang, Lei Yang, John Drennan, and Jin Zou*

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Impact of Chemical Heterogeneity on the Accuracy of Pore Size Distributions in Disordered Solids
Iain Hitchcock,* Shoaib Malik, Elizabeth M. Holt, Robin S. Fletcher, and Sean P. Bigby*

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Quantitative Dynamics and Structure for Crystalline Cs₂WO₄ and KMnO₄ Determined from High-Field ¹⁷O Variable-Temperature MAS NMR Experiments
Hans J. Jakobsen,* Henrik Bildsøe, Michael Brorson, Zhehong Gan, and Ivan Hung

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Electron Paramagnetic Resonance Tracing of Electronic Transfers in Push–Pull Copolymers/PCBM or Nanocrystal Composites
B. Pépin-Donat,* C. Ottone, Christophe Morell, C. Lombard, A. Lefrançois, P. Reiss, M. Leclerc, and S. Sadki

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X. W. Zhou,* M. E. Foster, F. B. van Swol, J. E. Martin, and Bryan M. Wong

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Oxidation at the Core–Ligand Interface of Au Lipoic Acid Nanoclusters That Enhances the Near-IR Luminescence
Jie Jiang, Cecil V. Conroy, Maksim M. Kvetny, Gabriel J. Lake, Jonathan W. Padelford, Tarushee Ahuja, and Gangli Wang*

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Dopamine Adsorption on TiO₂ Anatase Surfaces
I. Urdaneta, A. Keller, O. Atabek, J. L. Palma, D. Finkelstein-Shapiro, P. Tarakeshwar, V. Mujica, and M. Calatayud*

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Influence of Charge States on the π – π Interactions of Aromatic Side Chains with Surface of Graphene Sheet and Single-Walled Carbon Nanotubes in Bioelectrodes
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Non-Radiative Electron–Hole Recombination in Silicon Clusters: Ab Initio Non-Adiabatic Molecular Dynamics
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