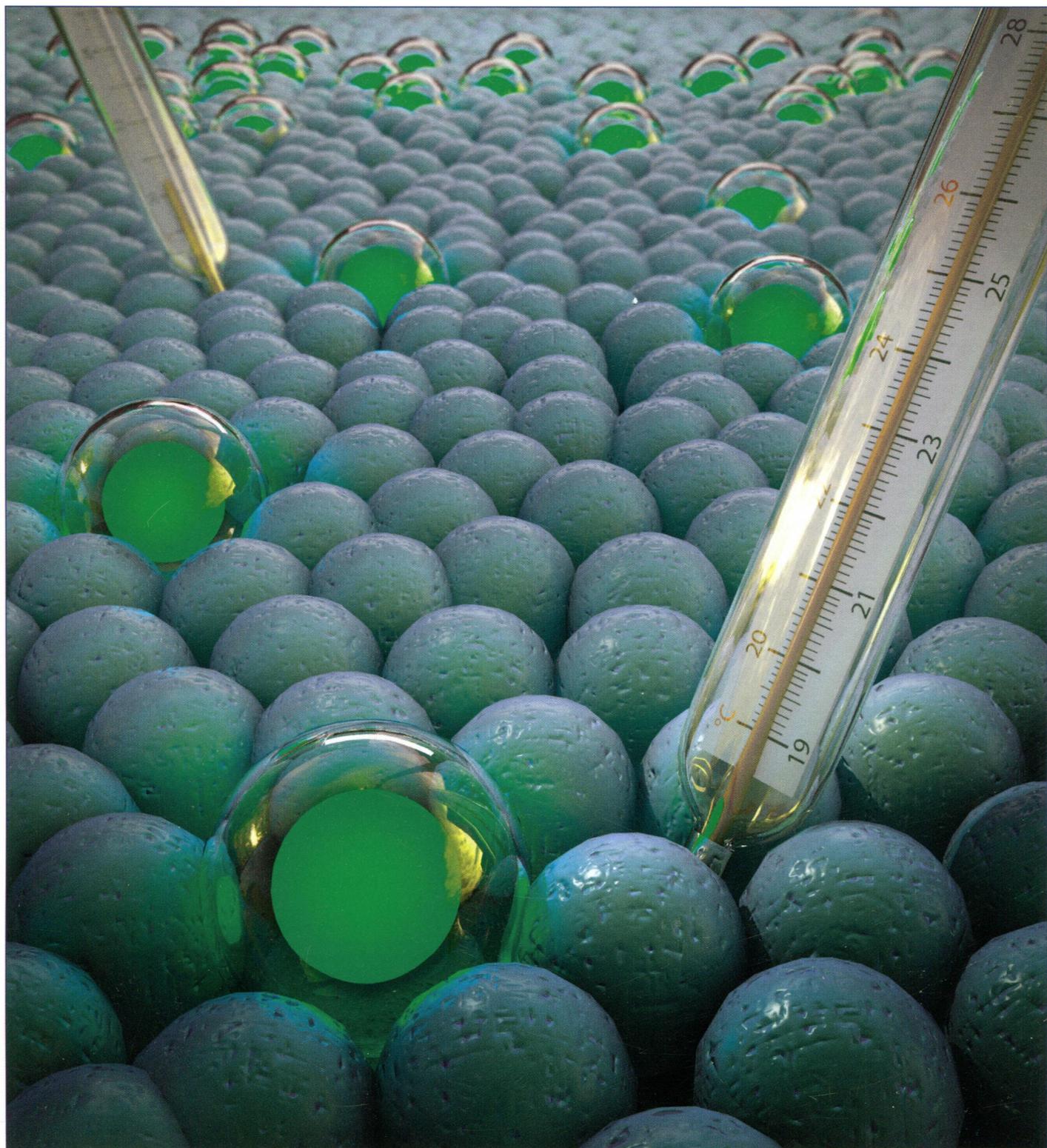


TW  
A 47/cs

November 12, 2014  
Volume 136  
Number 45  
pubs.acs.org/JACS

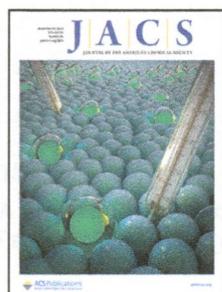
# J | A | C | S

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY



ACS Publications  
Most Trusted. Most Cited. Most Read.

[www.acs.org](http://www.acs.org)



**ON THE COVER:** Modern biology requires measurements inside the crowded environment of living cells. The spheres represent the cytoplasm of a cell where thermophoresis is measured for the first time. Previously, thermophoresis, the movement of molecules along a temperature gradient, has been used to measure binding affinities. See Braun and Reichl, p 15955.

## Spotlights

15807

Spotlights on Recent JACS Publications  
ACS Contributing Correspondents\*

DOI: 10.1021/ja511195g



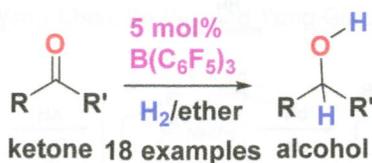
## Communications

15809



Enabling Catalytic Ketone Hydrogenation by Frustrated Lewis Pairs  
Tayseer Mahdi and Douglas W. Stephan\*

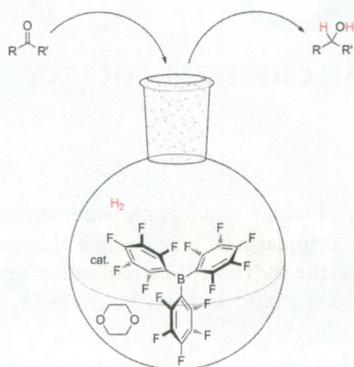
DOI: 10.1021/ja508829x



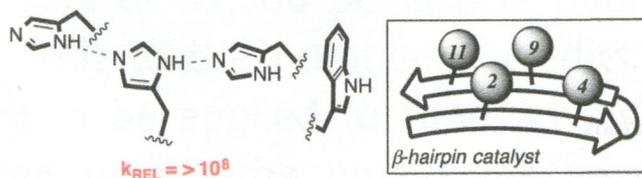
**METAL-FREE CATALYTIC  
HYDROGENATION**

## Nonmetal Catalyzed Hydrogenation of Carbonyl Compounds

Daniel J. Scott, Matthew J. Fuchter, and Andrew E. Ashley\*

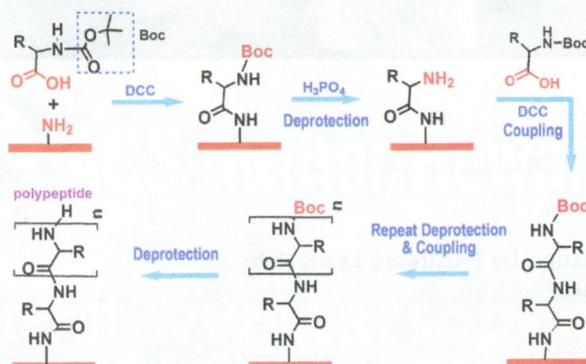
A Catalyst Selection Protocol That Identifies Biomimetic Motifs from  $\beta$ -Hairpin Libraries

Masaomi Matsumoto, Stephen J. Lee, Marcey L. Waters,\* and Michel R. Gagné\*



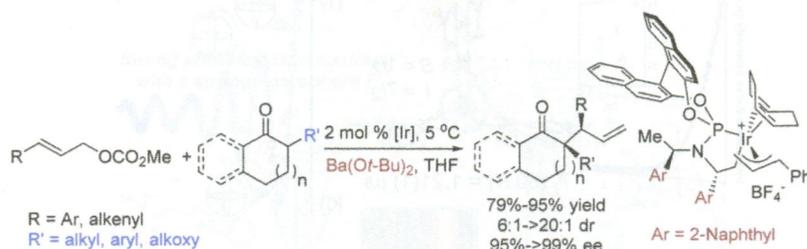
## Atomic Layer Deposition of L-Alanine Polypeptide

Yaqin Fu, Binsong Li, Ying-Bing Jiang,\* Darren R. Dunphy, Andy Tsai, Siu-Yue Tam, Hongyou Fan, Hongxia Zhang, David Rogers, Susan Rempe, Plamen Atanassov, Joseph L. Cecchi, and C. Jeffrey Brinker\*



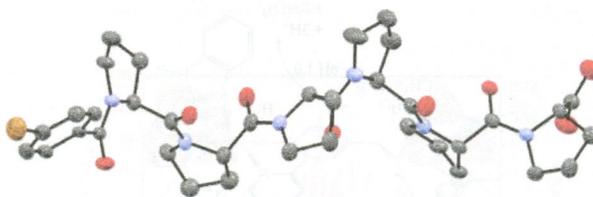
### Diastereo- and Enantioselective Iridium-Catalyzed Allylation of Cyclic Ketone Enolates: Synergistic Effect of Ligands and Barium Enolates

Wenyong Chen, Ming Chen, and John F. Hartwig\*



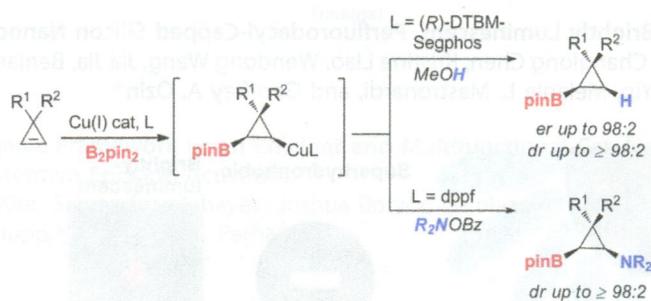
### A Crystal Structure of an Oligoproline PPII-Helix, at Last

Patrick Wilhelm, Bartosz Lewandowski, Nils Trapp, and Helma Wennemers\*



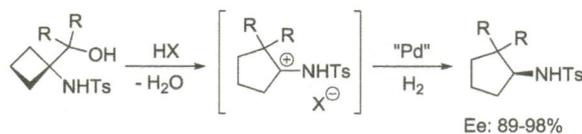
### Copper-Catalyzed Diastereo- and Enantioselective Desymmetrization of Cyclopropenes: Synthesis of Cyclopropylboronates

Alejandro Parra, Laura Amenós, Manuel Guisán-Ceinos, Aurora López, José Luis García Ruano, and Mariola Tortosa\*



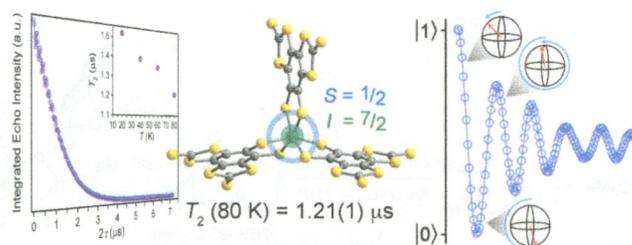
### Asymmetric Hydrogenation via Capture of Active Intermediates Generated from Aza-Pinacol Rearrangement

Chang-Bin Yu, Wen-Xue Huang, Lei Shi, Mu-Wang Chen, Bo Wu, and Yong-Gui Zhou\*

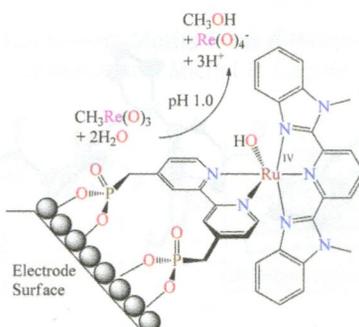


## Multiple Quantum Coherences from Hyperfine Transitions in a Vanadium(IV) Complex

Joseph M. Zadrozny, Jens Niklas, Oleg G. Poluektov, and Danna E. Freedman\*

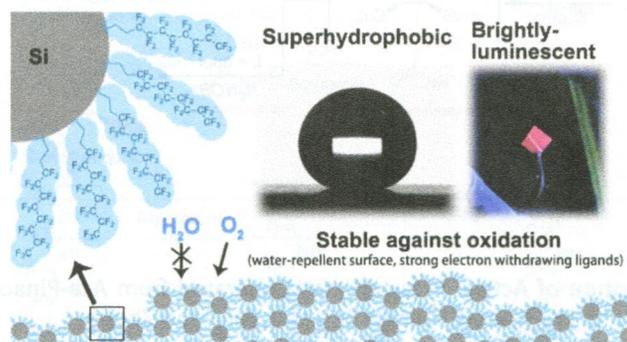
Selective Electrocatalytic Oxidation of a Re–Methyl Complex to Methanol by a Surface-Bound Ru<sup>II</sup> Polypyridyl Catalyst

Michael K. Coggins, Manuel A. Méndez, Javier J. Concepcion, Roy A. Periana, and Thomas J. Meyer\*



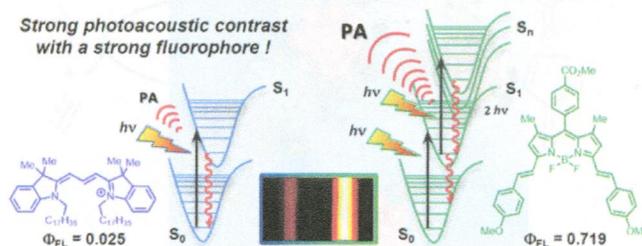
## Non-wettable, Oxidation-Stable, Brightly Luminescent, Perfluorodecyl-Capped Silicon Nanocrystal Film

Chenxi Qian, Wei Sun, Liwei Wang, Changlong Chen, Kristine Liao, Wendong Wang, Jia Jia, Benjamin D. Hatton, Gilberto Casillas, Marty Kurylowicz, Christopher M. Yip, Melanie L. Mastronardi, and Geoffrey A. Ozin\*



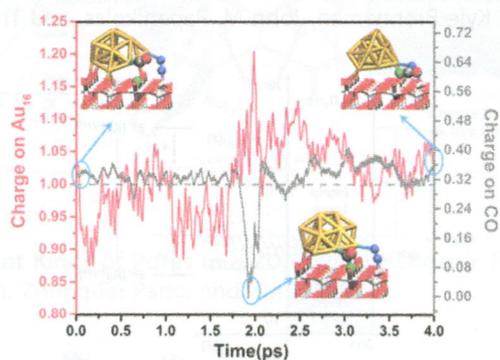
## Shining Light on the Dark Side of Imaging: Excited State Absorption Enhancement of a Bis-styryl BODIPY Photoacoustic Contrast Agent

Mathieu Frenette, Maryam Hatamimoslehabadi, Stephanie Bellinger-Buckley, Samir Laoui, Jeffrey La, Seema Bag, Srivalleesha Mallidi, Tayyaba Hasan, Brett Bouma, Chandra Yelleswarapu,\* and Jonathan Rochford\*



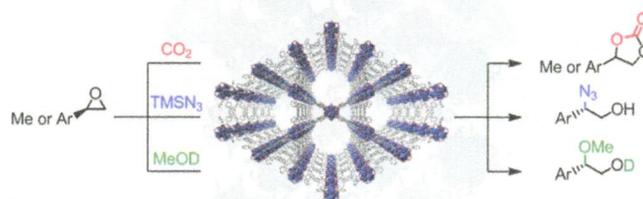
## Direct Simulation Evidence of Generation of Oxygen Vacancies at the Golden Cage Au<sub>16</sub> and TiO<sub>2</sub> (110) Interface for CO Oxidation

Lei Li and Xiao Cheng Zeng\*



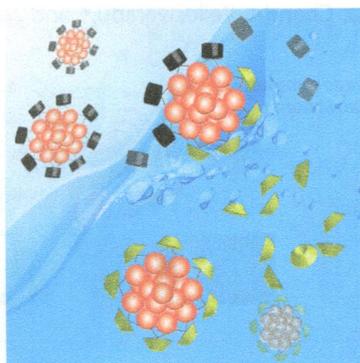
## A Hafnium-Based Metal–Organic Framework as an Efficient and Multifunctional Catalyst for Facile CO<sub>2</sub> Fixation and Regioselective and Enantioselective Epoxide Activation

M. Hassan Beyzavi, Rachel C. Klet, Samat Tussupbayev, Joshua Borycz, Nicolaas A. Vermeulen, Christopher J. Cramer, J. Fraser Stoddart, Joseph T. Hupp,\* and Omar K. Farha\*



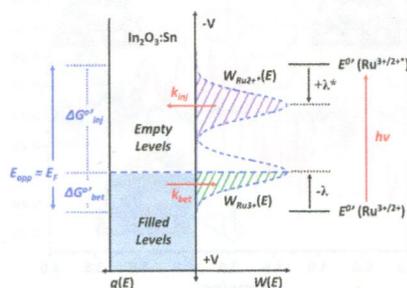
### Neat and Complete: Thiolate-Ligand Exchange on a Silver Molecular Nanoparticle

Lina G. AbdulHalim, Nuwan Kothalawala, Lutfan Sinatra, Amala Dass, and Osman M. Bakr\*



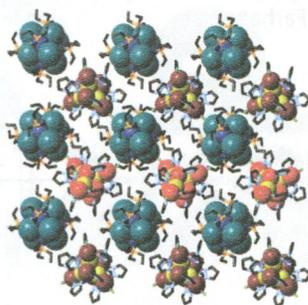
### Driving Force Dependent, Photoinduced Electron Transfer at Degenerately Doped, Optically Transparent Semiconductor Nanoparticle Interfaces

Byron H. Farnum, Zachary A. Morseth, M. Kyle Brennaman, John M. Papanikolas, and Thomas J. Meyer\*



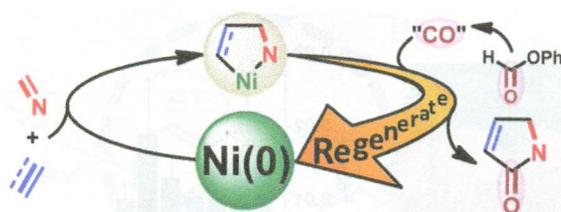
### Assembling Hierarchical Cluster Solids with Atomic Precision

Ari Turkiewicz, Daniel W. Paley, Tiglet Besara, Giselle Elbaz, Andrew Pinkard, Theo Siegrist, and Xavier Roy\*



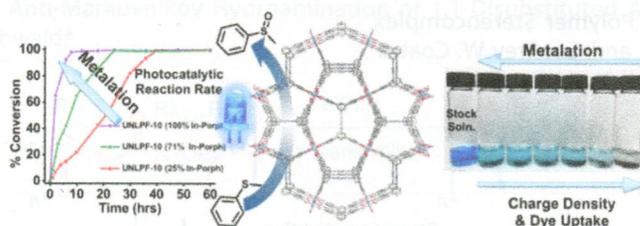
Nickel(0)-Catalyzed [2 + 2 + 1] Carbonylative Cycloaddition of Imines and Alkynes or Norbornene Leading to  $\gamma$ -Lactams

Yoichi Hoshimoto, Tomoya Ohata, Yukari Sasaoka, Masato Ohashi, and Sensuke Ogoshi\*



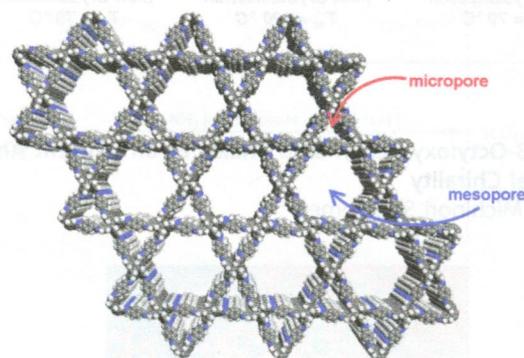
## Facile Control of the Charge Density and Photocatalytic Activity of an Anionic Indium Porphyrin Framework via in Situ Metalation

Jacob A. Johnson, Xu Zhang, Tyler C. Reeson, Yu-Sheng Chen, and Jian Zhang\*

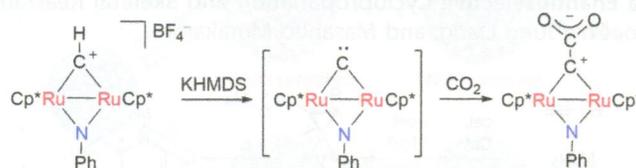


## One-Step Construction of Two Different Kinds of Pores in a 2D Covalent Organic Framework

Tian-You Zhou, Shun-Qi Xu, Qiang Wen, Zhong-Fu Pang, and Xin Zhao\*

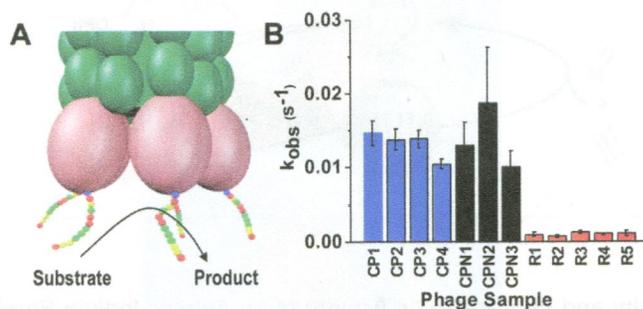
A Diruthenium  $\mu$ -Carbido Complex That Shows Singlet-Carbene-like Reactivity

Shin Takemoto,\* Jun Ohata, Kento Umetani, Masahiro Yamaguchi, and Hiroyuki Matsuzaka\*



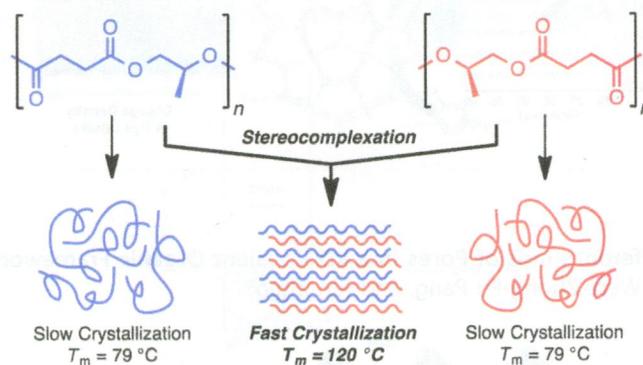
## Discovery of Catalytic Phages by Biocatalytic Self-Assembly

Yoshiaki Maeda, Nadeem Javid, Krystyna Duncan, Louise Birchall, Kirsty F. Gibson, Daniel Cannon, Yuka Kanetsuki, Charles Knapp, Tell Tuttle, Rein V. Ulijn,\* and Hiroshi Matsui\*



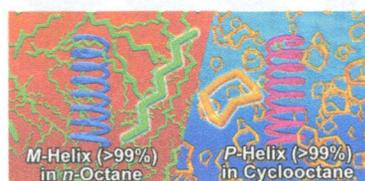
## Poly(propylene succinate): A New Polymer Stereocomplex

Julie M. Longo, Angela M. DiCiccio, and Geoffrey W. Coates\*

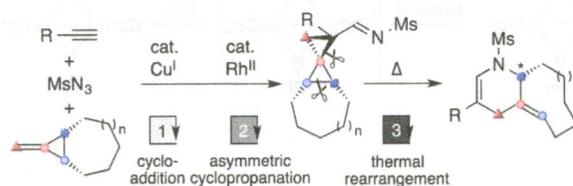


## Poly(quinoxaline-2,3-diyl)s Bearing (S)-3-Octyloxymethyl Side Chains as an Efficient Amplifier of Alkane Solvent Effect Leading to Switch of Main-Chain Helical Chirality

Yuuya Nagata, Tsuyoshi Nishikawa, and Michinori Sugimoto\*

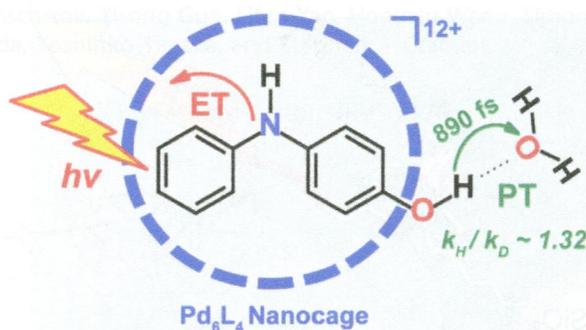
Synthesis of *trans*-Cycloalkenes via Enantioselective Cyclopropanation and Skeletal Rearrangement

Tomoya Miura,\* Takayuki Nakamuro, Chia-Jung Liang, and Masahiro Murakami\*



## Light-Induced Proton-Coupled Electron Transfer Inside a Nanocage

Rahul Gera, Ankita Das, Ajay Jha, and Jyotishman Dasgupta\*



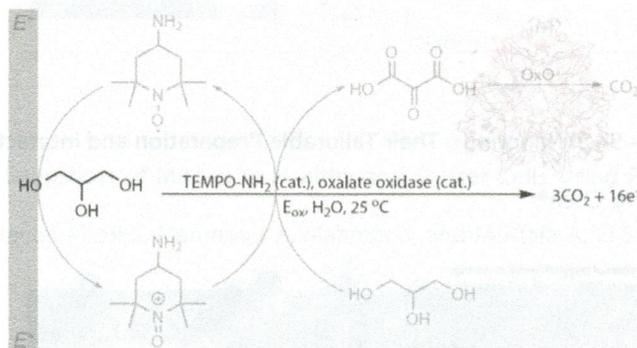
## Enantioselective CuH-Catalyzed Anti-Markovnikov Hydroamination of 1,1-Disubstituted Alkenes

Shaolin Zhu and Stephen L. Buchwald\*



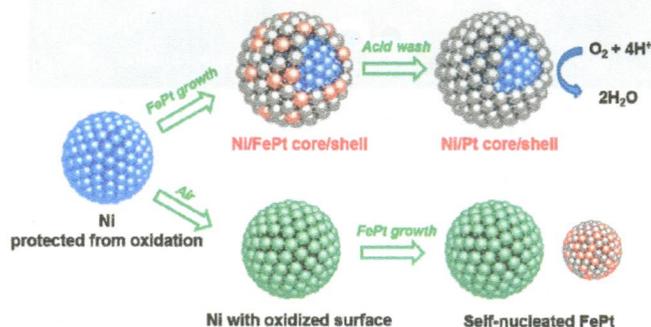
## Hybrid Enzymatic and Organic Electrocatalytic Cascade for the Complete Oxidation of Glycerol

David P. Hickey, Matthew S. McCammant, Fabien Giroud, Matthew S. Sigman,\* and Shelley D. Minteer\*



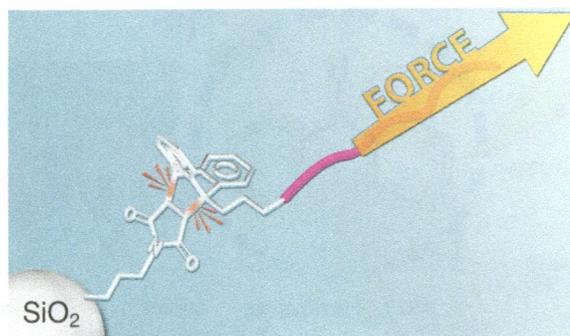
## Monodisperse Core/Shell Ni/FePt Nanoparticles and Their Conversion to Ni/Pt to Catalyze Oxygen Reduction

Sen Zhang, Yizhou Hao, Dong Su, Vicky V. T. Doan-Nguyen, Yaoting Wu, Jing Li, Shouheng Sun, and Christopher B. Murray\*

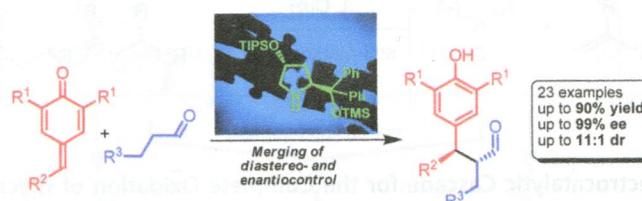


## Mechanophore Activation at Heterointerfaces

Jun Li, Tomohiro Shiraki, Bin Hu, Roger A. E. Wright, Bin Zhao, and Jeffrey S. Moore\*

A New Organocatalytic Concept for Asymmetric  $\alpha$ -Alkylation of Aldehydes

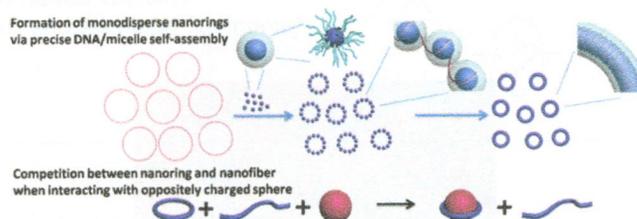
Lorenzo Caruana, Florian Kniep, Tore Küllerich Johansen, Pernille H. Poulsen, and Karl Anker Jørgensen\*



## Articles

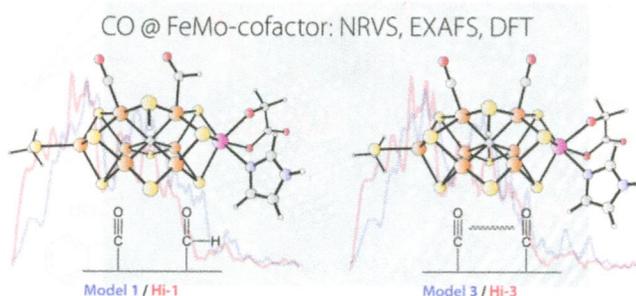
## Water-Soluble Monodisperse Core–Shell Nanorings: Their Tailorable Preparation and Interactions with Oppositely Charged Spheres of a Similar Diameter

Kaka Zhang, Han Miao, and Daoyong Chen\*



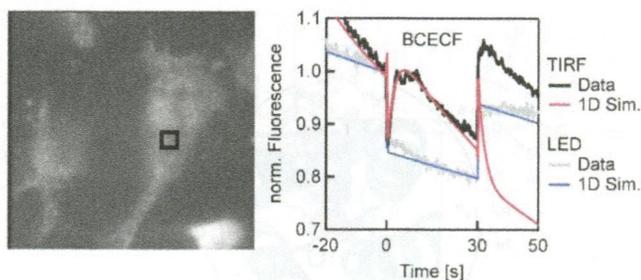
### Structural Characterization of CO-Inhibited Mo-Nitrogenase by Combined Application of Nuclear Resonance Vibrational Spectroscopy, Extended X-ray Absorption Fine Structure, and Density Functional Theory: New Insights into the Effects of CO Binding and the Role of the Interstitial Atom

Aubrey D. Scott, Vladimir Pelmenschikov, Yisong Guo, Lifen Yan, Hongxin Wang, Simon J. George, Christie H. Dapper, William E. Newton, Yoshitaka Yoda, Yoshihito Tanaka, and Stephen P. Cramer\*



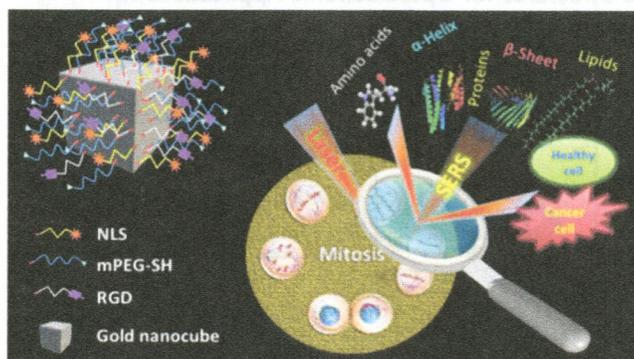
### Thermophoretic Manipulation of Molecules inside Living Cells

Maren R. Reichl and Dieter Braun\*



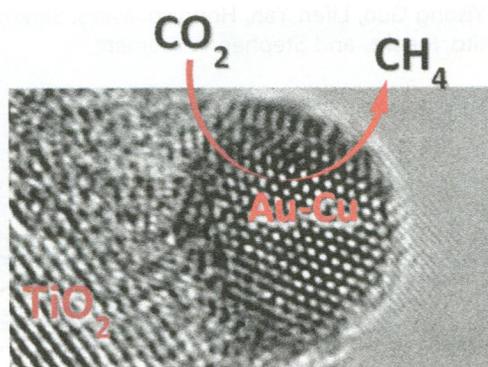
### Unraveling the Biomolecular Snapshots of Mitosis in Healthy and Cancer Cells Using Plasmonically-Enhanced Raman Spectroscopy

Sajanlal R. Panikkanvalappil, Steven M. Hira, Mahmoud A. Mahmoud, and Mostafa A. El-Sayed\*



Gold–Copper Nanoalloys Supported on TiO<sub>2</sub> as Photocatalysts for CO<sub>2</sub> Reduction by Water

Ștefan Neațu, Juan Antonio Maciá-Agulló, Patricia Concepción, and Hermenegildo Garcia\*

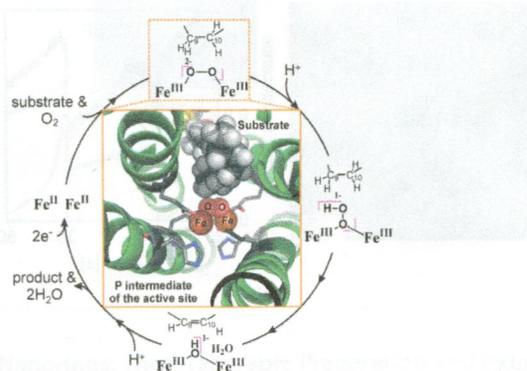


15977

DOI: 10.1021/ja506934k

Reactivity of the Binuclear Non-Heme Iron Active Site of  $\Delta^9$  Desaturase Studied by Large-Scale Multireference *Ab Initio* Calculations

Jakub Chalupský, Tibor András Rokob, Yuki Kurashige, Takeshi Yanai, Edward I. Solomon,\* Lubomír Rulíšek,\* and Martin Srnc\*

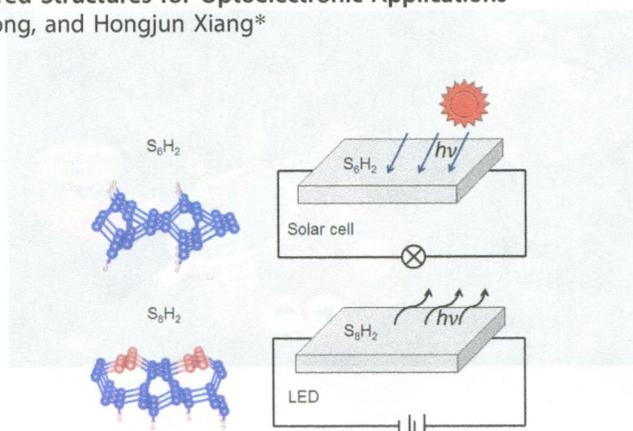


15992

DOI: 10.1021/ja507147p

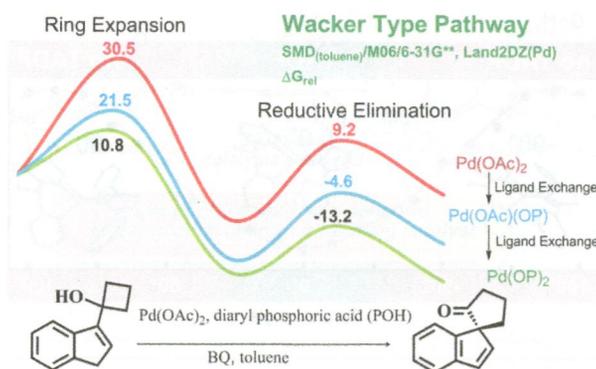
## Prediction of Silicon-Based Layered Structures for Optoelectronic Applications

Wei Luo, Yanming Ma, Xingao Gong, and Hongjun Xiang\*



## Importance of Ligand Exchanges in Pd(II)-Brønsted Acid Cooperative Catalytic Approach to Spirocyclic Rings

Garima Jindal and Raghavan B. Sunoj\*

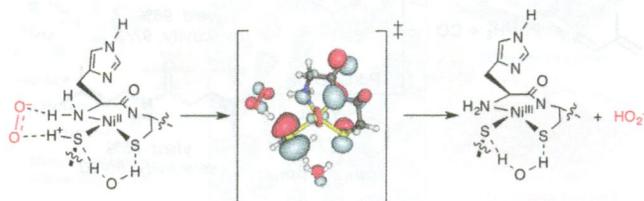


16009

DOI: 10.1021/ja5079514

## Cysteinate Protonation and Water Hydrogen Bonding at the Active-Site of a Nickel Superoxide Dismutase Metallopeptide-Based Mimic: Implications for the Mechanism of Superoxide Reduction

Jason Shearer,\* Kristy L. Peck, Jennifer C. Schmitt, and Kosh P. Neupane

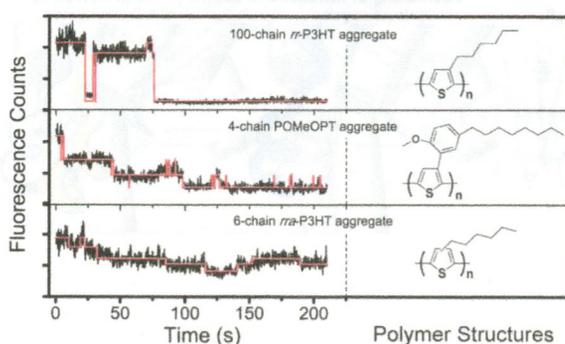


16023

DOI: 10.1021/ja508112k

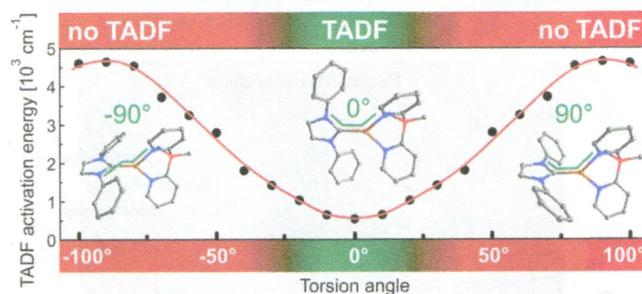
## Excitonic Energy Migration in Conjugated Polymers: The Critical Role of Interchain Morphology

Zhongjian Hu, Takuji Adachi, Ryan Haws, Bo Shuang, Robert J. Ono, Christopher W. Bielawski, Christy F. Landes, Peter J. Rossky, and David A. Vanden Bout\*



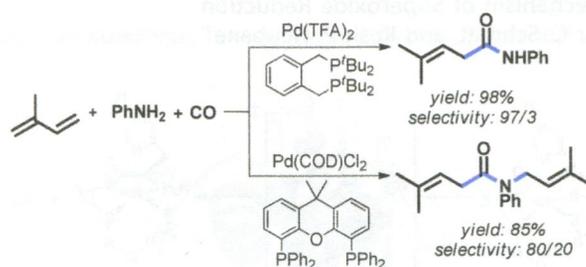
### Phosphorescence versus Thermally Activated Delayed Fluorescence. Controlling Singlet–Triplet Splitting in Brightly Emitting and Sublimable Cu(I) Compounds

Markus J. Leitl, Valentina A. Krylova, Peter I. Djurovich, Mark E. Thompson,\* and Hartmut Yersin\*



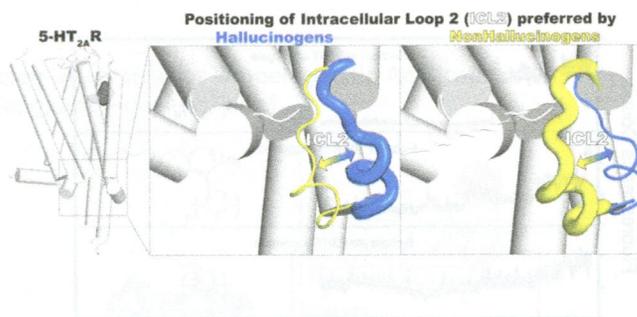
### Selective Palladium-Catalyzed Aminocarbonylation of 1,3-Dienes: Atom-Efficient Synthesis of $\beta,\gamma$ -Unsaturated Amides

Xianjie Fang, Haoquan Li, Ralf Jackstell, and Matthias Beller\*



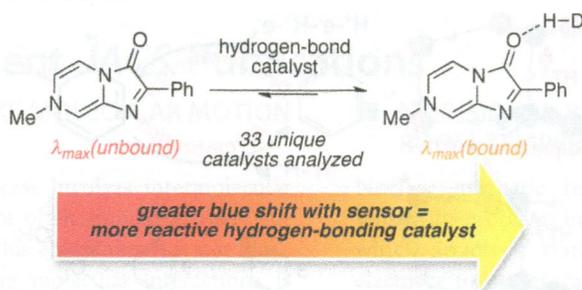
### A Functional Selectivity Mechanism at the Serotonin-2A GPCR Involves Ligand-Dependent Conformations of Intracellular Loop 2

Jose Manuel Perez-Aguilar, Jufang Shan, Michael V. LeVine, George Khelashvili, and Harel Weinstein\*



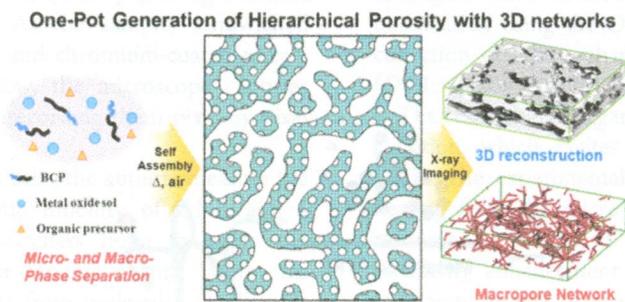
## Quantification of Electrophilic Activation by Hydrogen-Bonding Organocatalysts

Ryan R. Walvoord, Phuong N. H. Huynh, and Marisa C. Kozlowski\*



## Direct Access to Hierarchically Porous Inorganic Oxide Materials with Three-Dimensionally Interconnected Networks

Jongkook Hwang, Changshin Jo, Kahyun Hur, Jun Lim, Seongseop Kim, and Jinwoo Lee\*



## Interconversion between Three Overstretched DNA Structures

Xinghua Zhang, Yuanyuan Qu, Hu Chen, Ioulia Rouzina, Shengli Zhang, Patrick S. Doyle,\* and Jie Yan\*

