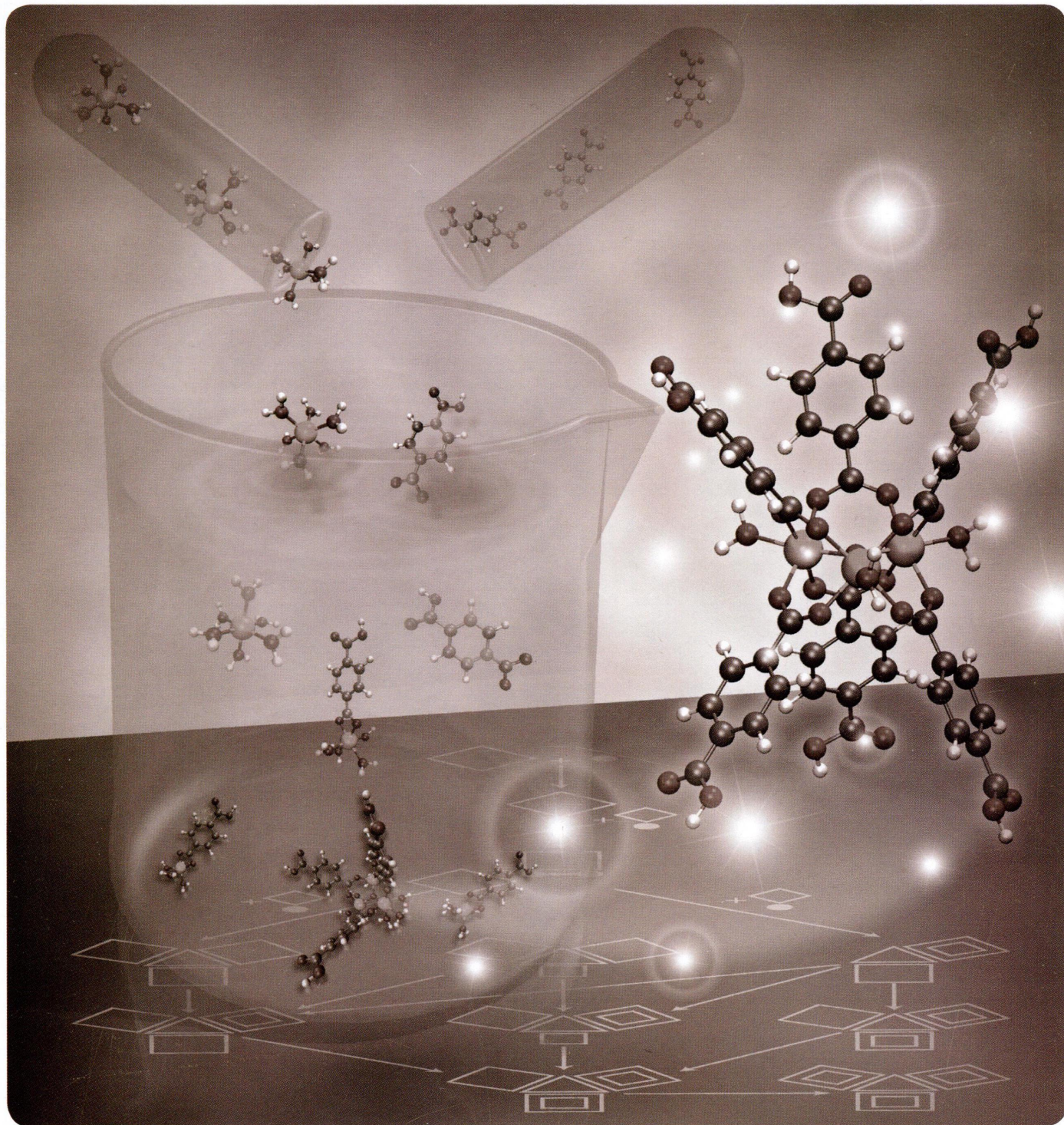


PM
C-51/9m

cm CHEMISTRY OF MATERIALS

NOVEMBER 25, 2014 | VOLUME 26 | NUMBER 22 | pubs.acs.org/cm



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

ON THE COVER: The development of rational synthetic strategies for metal–organic frameworks (MOFs) remains a challenge for this important class of materials. State-of-the-art molecular simulations were applied to uncover the individual elementary reaction steps leading to the self-assembly of secondary building units formed during hydrothermal synthesis of MOF MIL-101. Metal–ligand coordination, exchange reactions, and metal core spin states were taken into account. A microkinetic reaction network model was used to predict cluster formation rates based on the lowest energy barrier pathways, which correlated well with experimentally measured nucleation rates. The cover art was jointly prepared by the authors and Cortland Johnson of Pacific Northwestern National Laboratory. For more information, see “Formation Mechanism of the Secondary Building Unit in a Chromium Terephthalate Metal–Organic Framework” by David C. Cantu, B. Peter McGrail, and Vassiliki-Alexandra Glezakou* (*Chem. Mater.* **2014**, *26*, 6401–6409).

Editorial

6319

Scientific Publishing as an Art
Jillian M. Buriak*

DOI: 10.1021/cm503928y

Articles

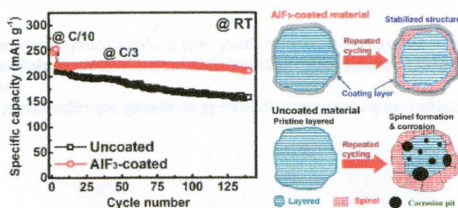
6320



Functioning Mechanism of AlF_3 Coating on the Li- and Mn-Rich Cathode Materials

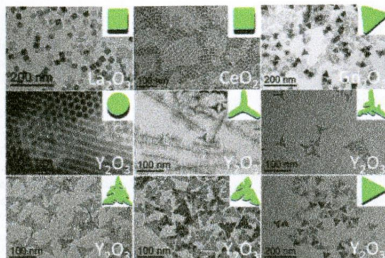
Jianming Zheng, Meng Gu, Jie Xiao, Bryant J. Polzin, Pengfei Yan, Xilin Chen, Chongmin Wang,* and Ji-Guang Zhang*

DOI: 10.1021/cm502071h



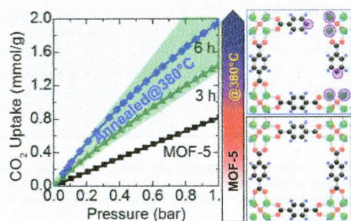
Mineralizer-Assisted Shape-Control of Rare Earth Oxide Nanoplates

Dianyuan Wang, Yijin Kang, Xingchen Ye, and Christopher B. Murray*



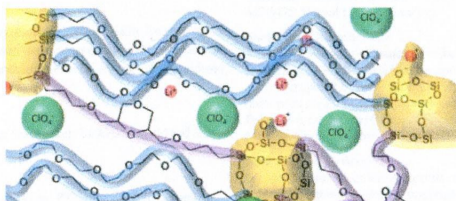
Postsynthesis Annealing of MOF-5 Remarkably Enhances the Framework Structural Stability and CO₂ Uptake

Srinivas Gadipelli* and Zhengxiao Guo*



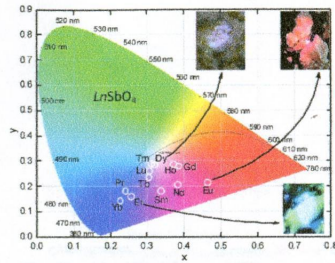
Highly Conducting 3D-Hybrid Polymer Electrolytes for Lithium Batteries Based on Siloxane Networks and Cross-Linked Organic Polar Interphases

Nicola Boaretto, Andreas Bittner, Christine Brinkmann, Birke-Elisabeth Olsowski, Jochen Schulz, Mona Seyfried, Keti Vezzù, Michael Popall, and Vito Di Noto*



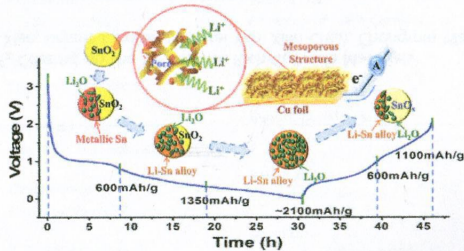
Lanthanide Orthoantimonate Light Emitters: Structural, Vibrational, and Optical Properties

Kisla P. F. Siqueira, Patrícia P. Lima, Rute A. S. Ferreira, Luís D. Carlos, Eduardo M. Bittar, Eduardo Granado, Juan Carlos González, Arturo Abelenda, Roberto L. Moreira, and Anderson Dias*



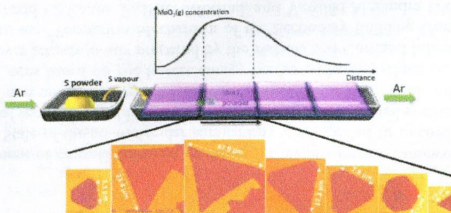
New Insight into the Reaction Mechanism for Exceptional Capacity of Ordered Mesoporous SnO_2 Electrodes via Synchrotron-Based X-ray Analysis

Hyunchul Kim, Gwi Ok Park, Yunok Kim, Shoab Muhammad, Jaeseung Yoo, Mahalingam Balasubramanian, Yong-Hun Cho, Min-Gyu Kim, Byungju Lee, Kisuk Kang, Hansu Kim,* Ji Man Kim,* and Won-Sub Yoon*

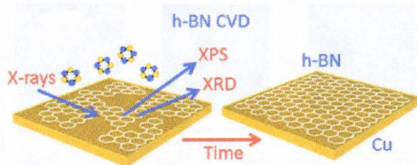


Shape Evolution of Monolayer MoS_2 Crystals Grown by Chemical Vapor Deposition

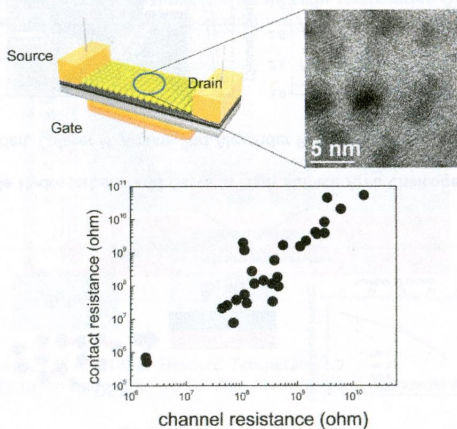
Shanshan Wang, Youmin Rong, Ye Fan, Mercè Pacios, Harish Bhaskaran, Kuang He, and Jamie H. Warner*



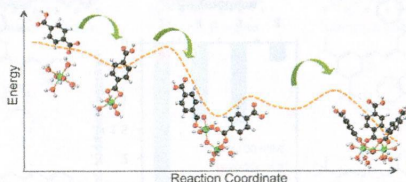
In Situ Observations during Chemical Vapor Deposition of Hexagonal Boron Nitride on Polycrystalline Copper
 Piran R. Kidambi, Raoul Blume, Jens Kling, Jakob B. Wagner, Carsten Baetz, Robert S. Weatherup, Robert Schloegl, Bernhard C. Bayer, and Stephan Hofmann*



Competition between Charge Transport and Energy Barrier in Injection-Limited Metal/Quantum Dot Nanocrystal Contacts
 Youngjun Kim, Seongeun Cho, Sunho Jeong, Doo-Hyun Ko, Hyungduk Ko, Namho You, Mincheol Chang, Elsa Reichmanis, Jun-Young Park, Sung Young Park, Jong Suk Lee,* Heesun Yang,* Insik In,* and Byoungnam Park*

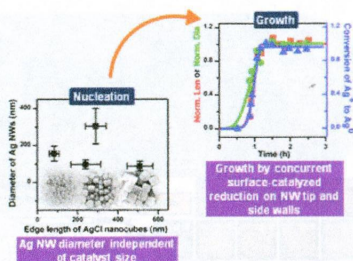


Formation Mechanism of the Secondary Building Unit in a Chromium Terephthalate Metal–Organic Framework
 David C. Cantu, B. Peter McGrail, and Vassiliki-Alexandra Glezakou*



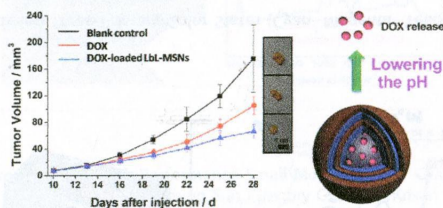
Polyol Synthesis of Silver Nanowires by Heterogeneous Nucleation; Mechanistic Aspects Influencing Nanowire Diameter and Length

Waynie M. Schuette and William E. Buhro*



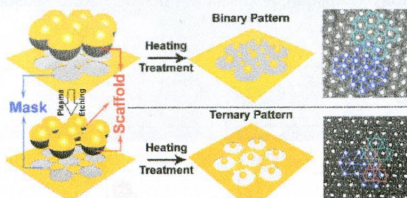
Mesoporous Silica Nanoparticles Coated by Layer-by-Layer Self-assembly Using Cucurbit[7]uril for in Vitro and in Vivo Anticancer Drug Release

Qing-Lan Li, Yanfang Sun, Yu-Long Sun, Jijie Wen, Yue Zhou, Qi-Ming Bing, Lyle D. Isaacs, Yinghua Jin, Hui Gao,* and Ying-Wei Yang*



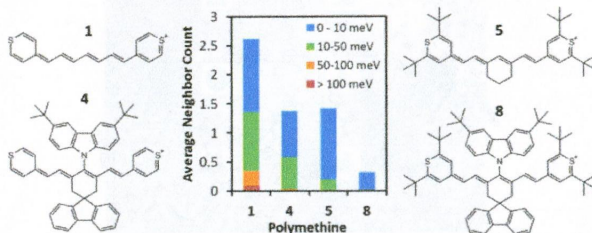
Combining the Masking and Scaffolding Modalities of Colloidal Crystal Templates: Plasmonic Nanoparticle Arrays with Multiple Periodicities

Shikuan Yang,* Daniel Slotcavage, John D. Mai, Wansheng Liang, Yuliang Xie, Yuchao Chen, and Tony Jun Huang*



Effect of Bulky Substituents on Thiopyrylium Polymethine Aggregation in the Solid State: A Theoretical Evaluation of the Implications for All-Optical Switching Applications

Rebecca L. Giesekeing, Sukrit Mukhopadhyay, Chad Risko, Seth R. Marder, and Jean-Luc Brédas*



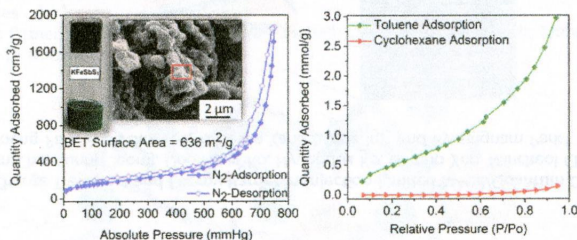
Enhancement of Initial Growth of ZnO Films on Layer-Structured Bi₂Te₃ by Atomic Layer Deposition

Kwang-Chon Kim, Cheol Jin Cho, Joohwi Lee, Hyun Jae Kim, Doo Seok Jeong, Seung-Hyub Baek, Jin-Sang Kim,* and Seong Keun Kim*



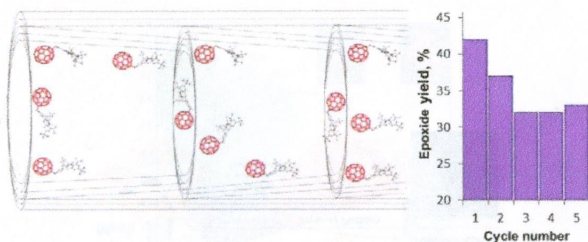
Selective Adsorption of Volatile Hydrocarbons and Gases in High Surface Area Chalcogels Containing [ES₃]³⁻ Anions (E = As, Sb)

Ejaz Ahmed, Jayaprakash Khanderi, Dalaver H. Anjum, and Alexander Rothenberger*



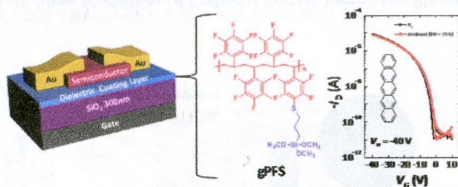
New Pathway for Heterogenization of Molecular Catalysts by Non-covalent Interactions with Carbon Nanoreactors

Maria A. Lebedeva, Thomas W. Chamberlain, Martin Schröder, and Andrei N. Khlobystov*



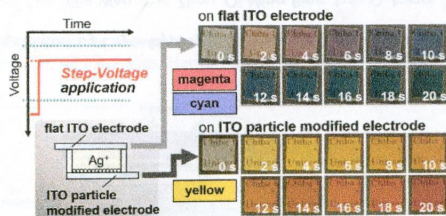
Grafting Fluorinated Polymer Nanolayer for Advancing the Electrical Stability of Organic Field-Effect Transistors

Kyunghun Kim, Tae Kyu An, Jiye Kim, Yong Jin Jeong, Jaeyoung Jang, Haekyung Kim, Jang Yeol Baek, Yun-Hi Kim,*
Se Hyun Kim,* and Chan Eon Park*



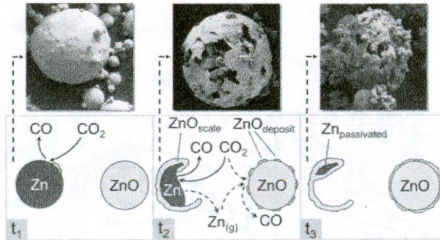
Multicolor Electrochromism Showing Three Primary Color States (Cyan–Magenta–Yellow) Based on Size- and Shape-Controlled Silver Nanoparticles

Ayako Tsuboi, Kazuki Nakamura, and Norihisa Kobayashi*



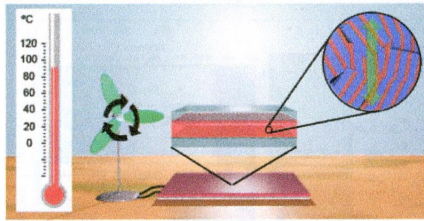
Mechanism of Zn Particle Oxidation by H₂O and CO₂ in the Presence of ZnO

David Weibel, Zoran R. Jovanovic,* Elena Gálvez, and Aldo Steinfeld



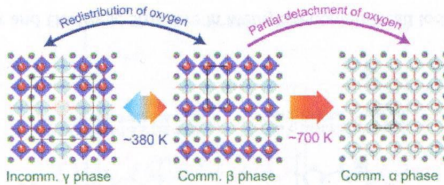
Nanostructured Two-Component Liquid-Crystalline Electrolytes for High-Temperature Dye-Sensitized Solar Cells

Daniel Högberg, Bartolome Soberats, Satoshi Uchida, Masafumi Yoshio, Lars Kloo, Hiroshi Segawa, and Takashi Kato*



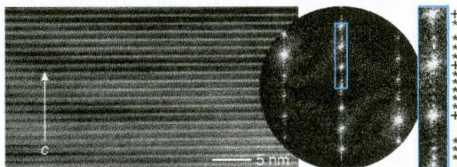
Structural Evolution of GdBaCo₂O_{5.6} ($\delta = 7/18$) at Elevated Temperatures

Nobuo Ishizawa,* Toru Asaka, Tatsunari Kudo, Koichiro Fukuda, Akira Yasuhara, Nobuyuki Abe, and Taka-hisa Arima



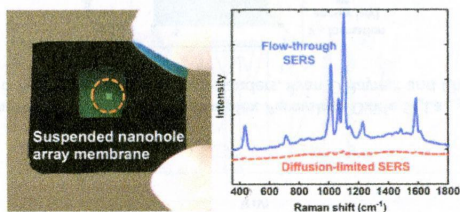
Synthesis and Thermal Instability of High-Quality $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$ Superlattice Thin Film Thermoelectrics

Anna-Lena Hansen, Torben Dankwort, Markus Winkler, Jeffrey Ditto, Dave C. Johnson, Jan D. Koenig, Kilian Bartholomé, Lorenz Kienle,* and Wolfgang Bensch*



Millimeter-Sized Suspended Plasmonic Nanohole Arrays for Surface-Tension-Driven Flow-Through SERS

Shailabh Kumar, Sudhir Cherukulappurath, Timothy W. Johnson, and Sang-Hyun Oh*



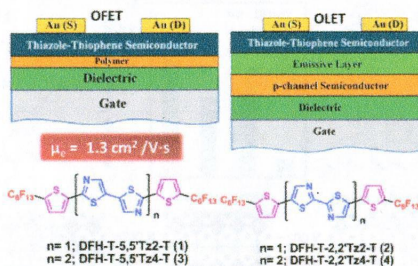
The Role of Solvent Additive Processing in High Performance Small Molecule Solar Cells

Louis A. Perez, James T. Rogers, Michael A. Brady, Yanming Sun, Gregory C. Welch, Kristin Schmidt, Michael F. Toney, Hiroshi Jinnai, Alan J. Heeger, Michael L. Chabynyc, Guillermo C. Bazan,* and Edward J. Kramer*



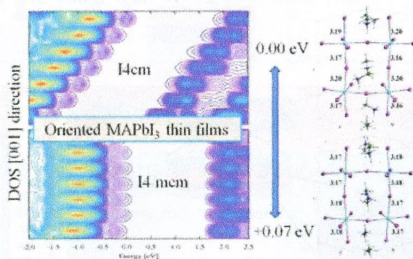
Perfluoroalkyl-Functionalized Thiazole–Thiophene Oligomers as N-Channel Semiconductors in Organic Field-Effect and Light-Emitting Transistors

Hakan Usta,* William Christopher Sheets, Mitchell Denti, Gianluca Generali, Raffaella Capelli, Shaofeng Lu, Xinge Yu, Michele Muccini,* and Antonio Facchetti*



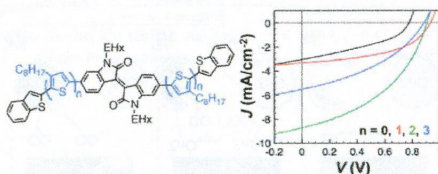
Interplay of Orientational Order and Electronic Structure in Methylammonium Lead Iodide: Implications for Solar Cell Operation

Claudio Quarti, Edoardo Mosconi, and Filippo De Angelis*



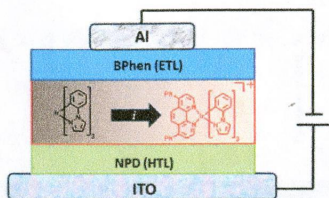
Isoindigo-Containing Molecular Semiconductors: Effect of Backbone Extension on Molecular Organization and Organic Solar Cell Performance

Yi Ren, Anna K. Hailey, Anna M. Hiszpanski, and Yueh-Lin Loo*



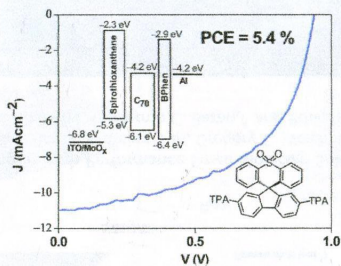
In Situ Observation of Degradation by Ligand Substitution in Small-Molecule Phosphorescent Organic Light-Emitting Diodes

Matthew J. Jurow, Alberto Bossi, Peter I. Djurovich, and Mark E. Thompson*



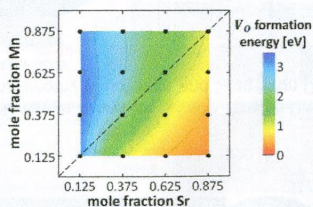
Hole-Transporting Spirothioxanthene Derivatives as Donor Materials for Efficient Small-Molecule-Based Organic Photovoltaic Devices

Chin-Yiu Chan, Yi-Chun Wong, Mei-Yee Chan,* Sin-Hang Cheung, Shu-Kong So, and Vivian Wing-Wah Yam*



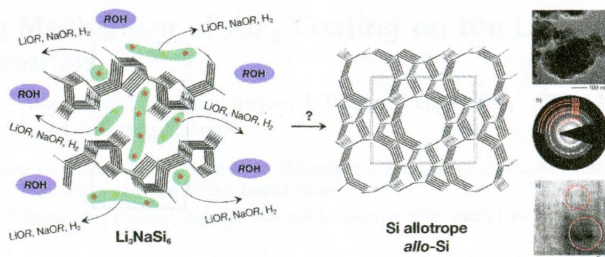
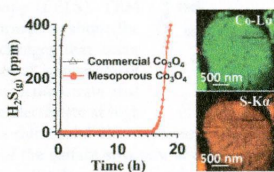
Tunable Oxygen Vacancy Formation Energetics in the Complex Perovskite Oxide $\text{Sr}_x\text{La}_{1-x}\text{Mn}_y\text{Al}_{1-y}\text{O}_3$

Ann M. Deml, Vladan Stevanović, Aaron M. Holder, Michael Sanders, Ryan O'Hayre,* and Charles B. Musgrave*



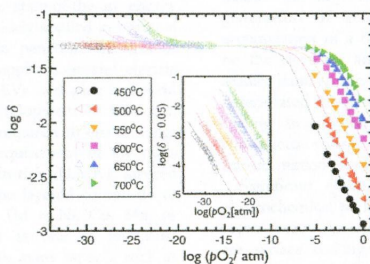
Alkali Metals Extraction Reactions with the Silicides $\text{Li}_{15}\text{Si}_4$ and Li_3NaSi_4 : Amorphous Si versus *allo*-Si

Michael Zeilinger, Laura-Alice Jantke, Lavinia M. Scherf, Florian J. Kiefer, Gero Neubüser, Lorenz Kienle, Antti J. Karttunen, Sumit Konar, Ulrich Häussermann, and Thomas F. Fässler*

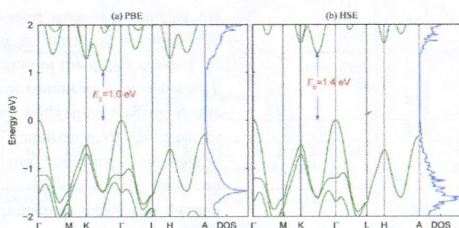
Low Temperature Desulfurization of H_2S : High Sorption Capacities by Mesoporous Cobalt Oxide via Increased H_2S Diffusion
Lakshitha R. Pahalagedara, Altug S. Poyraz, Wenqiao Song, Chung-Hao Kuo, Madhavi N. Pahalagedara, Yong-Tao Meng, and Steven L. Suib*

Nonstoichiometry in Oxide Thin Films Operating under Anodic Conditions: A Chemical Capacitance Study of the Praseodymium–Cerium Oxide System

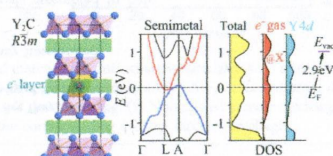
Di Chen, Sean R. Bishop, and Harry L. Tuller*



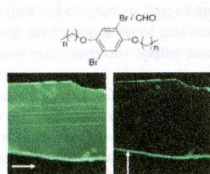
WS₂ As an Excellent High-Temperature Thermoelectric Material

Appala Naidu Gandhi and Udo Schwingenschlög^{*}

Two-Dimensional Transition-Metal Electride Y₂C

Xiao Zhang, Zewen Xiao, Hechang Lei, Yoshitake Toda, Satoru Matsuishi, Toshio Kamiya, Shigenori Ueda, and Hideo Hosono^{*}

Tuning the Photophysical Properties of Metal-Free Room Temperature Organic Phosphors via Compositional Variations in Bromobenzaldehyde/Dibromobenzene Mixed Crystals

Onas Bolton, Dongwook Lee, Jaehun Jung, and Jinsang Kim^{*}

	Br5	Br6	Br7	Br8
w/o emitter	0%	0%	0%	0%
Br5A	45%	43%	31%	23%
Br6A	36%	59%	49%	29%
Br7A	18%	29%	45%	33%
Br8A	9%	13%	37%	51%