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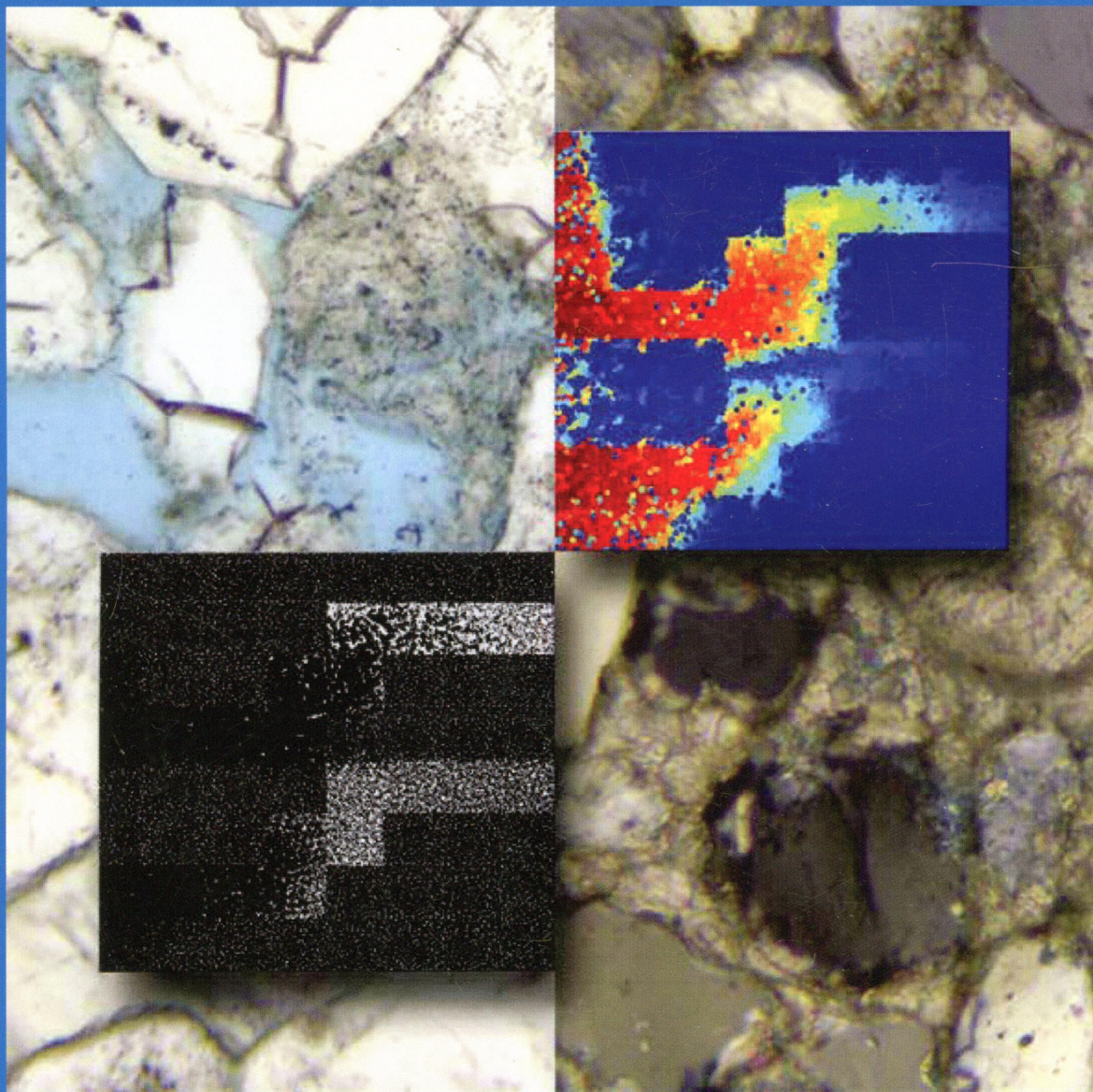
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# THE JOURNAL OF PHYSICAL CHEMISTRY

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Integrating  
Experiments,  
Simulations, and  
Natural Analog Site  
Analyses for  
Security of Geological  
CO<sub>2</sub> Storage  
(see page 15103)

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



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**ON THE COVER:** Integrating experiments, simulations, and natural analog site analyses for security of geological CO<sub>2</sub> storage. Research at the Center for Frontiers of Subsurface Energy Security (CFSES), a Department of Energy, Energy Frontier Research Center, provides insights into the geological CO<sub>2</sub> storage process. The background images are photomicrographs of unaltered (left) and altered (right) sandstone in the vicinity of a natural CO<sub>2</sub> seepage conduit at Little Grand Wash fault in Utah, USA. Primary porosity (blue) has been completely occluded in the altered sandstone by carbonate pore cement that precipitated from upward migrating CO<sub>2</sub>-charged brine. The negative feedback between focused fluid flow and calcite cementation contributes to the tendency of preferred flow pathways to migrate in space and time. Overset images show cementation (left) and normalized concentration (right) fields from multiscale reactive transport simulations that capture emergent behavior resulting from coupling of convection and reaction on the pore scale. This analysis provides quantitative insight into mechanisms for redirection of escape pathways due to pore plugging, as observed at Little Grand Wash fault. (Modified after multiple figures in Mehmani, Y.; Sun, T.; Balhoff, M. T.; Eichhubl, P.; Bryant, S. Multiblock Pore-Scale Modeling and Upscaling of Reactive Transport: Application to Carbon Sequestration. *Transp. Porous Media* 2012, 95, 305–326, with kind permission from Springer Science and Business Media.) See page 15103.

## Feature Article

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[dx.doi.org/10.1021/jp5006764](http://dx.doi.org/10.1021/jp5006764)

### Chemical and Hydrodynamic Mechanisms for Long-Term Geological Carbon Storage

Susan J. Altman,\* Behdad Aminzadeh, Matthew T. Balhoff, Philip C. Bennett, Steven L. Bryant, M. Bayani Cardenas, Kuldeep Chaudhary, Randall T. Cygan, Wen Deng, Thomas Dewers, David A. DiCarlo, Peter Eichhubl, Marc A. Hesse, Chun Huh, Edward N. Matteo, Yashar Mehmani, Craig M. Tenney, and Hongkyu Yoon

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[dx.doi.org/10.1021/jp5013494](http://dx.doi.org/10.1021/jp5013494)

Electrochemical Quartz Crystal Microbalance Analysis of Nitrogen Oxide-Promoted Platinum Dissolution in HClO<sub>4</sub>  
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[dx.doi.org/10.1021/jp502045w](http://dx.doi.org/10.1021/jp502045w)

Electronic and Optical Property Analysis of the Cu–Sb–S Tetrahedrites for High-Efficiency Absorption Devices  
C. Tablero\*

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[dx.doi.org/10.1021/jp5025087](http://dx.doi.org/10.1021/jp5025087)

Direct Electrical Evidence of Plasmonic Near-Field Enhancement in Small Molecule Organic Solar Cells  
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[dx.doi.org/10.1021/jp5037926](https://doi.org/10.1021/jp5037926)**Structural and Vibrational Properties of CdAl<sub>2</sub>S<sub>4</sub> under High Pressure: Experimental and Theoretical Approach**

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[dx.doi.org/10.1021/jp5039909](https://doi.org/10.1021/jp5039909)**Local Structure and Spin State of Cobalt Ion at Defect in Lithium Overstoichiometric LiCoO<sub>2</sub> As Studied by <sup>6,7</sup>Li Solid-State NMR Spectroscopy**

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[dx.doi.org/10.1021/jp5040739](https://doi.org/10.1021/jp5040739)**Synthesis and Spectroscopic Properties of Monoclinic  $\alpha$ -Eu<sub>2</sub>(MoO<sub>4</sub>)<sub>3</sub>**

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[dx.doi.org/10.1021/jp500349d](https://doi.org/10.1021/jp500349d)**Nitriding of Nanocrystalline Iron in the Atmospheres with Variable Nitriding Potential**

Dariusz Moszyński\*

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[dx.doi.org/10.1021/jp501642j](https://doi.org/10.1021/jp501642j)**Digital 3D Local Growth of Iron Oxide Micro- and Nanorods by Laser-Induced Photothermal Chemical Liquid Growth**

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**Molecular Dynamics Simulation of PEGylated Membranes with Cholesterol: Building Toward the DOXIL Formulation**  
Aniket Magarkar, Tomasz Róg, and Alex Bunker\*

## Additions and Corrections

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[dx.doi.org/10.1021/jp506235j](https://doi.org/10.1021/jp506235j)

**Correction to "Mechanistic Insights into the Formation of Dodecanethiolate-Stabilized Magnetic Iridium Nanoparticles: Thiosulfate vs Thiol Ligands"**

Diego J. Gavia, Yeonjin Do, Jiyeong Gu, and Young-Seok Shon\*