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J80/pa2

APRIL 3, 2014

VOLUME 118

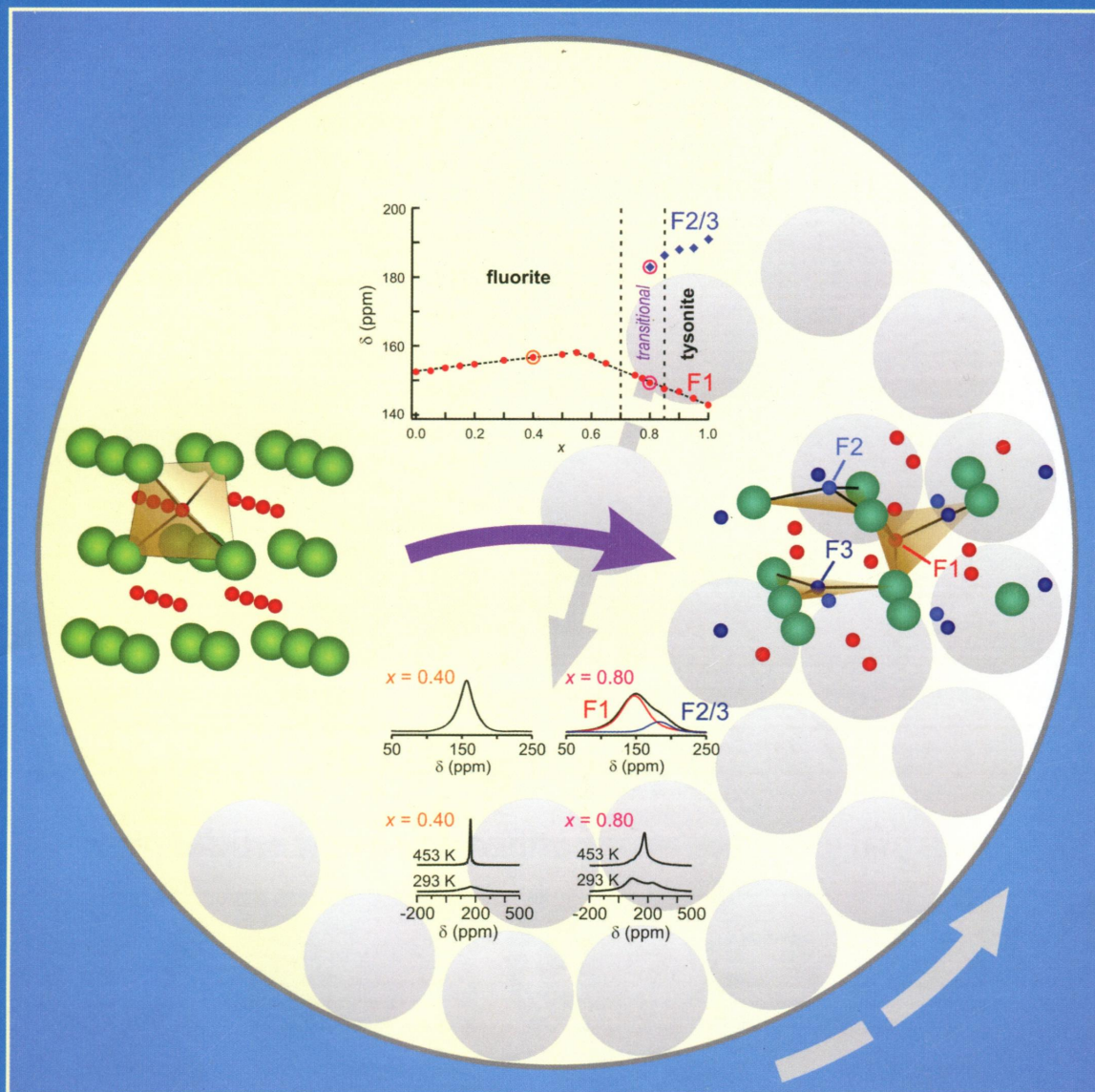
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# THE JOURNAL OF PHYSICAL CHEMISTRY

# C

Continuous Structural  
Transition of  
Mechanosynthesized  
 $Ba_{1-x}La_xF_{2+x}$  and  $F^-$   
Mobility Revealed  
by  $^{19}F$  NMR  
(see page 7117)



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**ON THE COVER:** Continuous structural transition of mechanothesized  $\text{Ba}_{1-x}\text{La}_x\text{F}_{2+x}$  and  $\text{F}^-$  mobility revealed by  $^{19}\text{F}$  NMR. The system  $\text{Ba}_{1-x}\text{La}_x\text{F}_{2+x}$  was mechanothesized for  $0 \leq x \leq 1$  by high-energy ball-milling mixtures of  $\text{BaF}_2$  and  $\text{LaF}_3$ . Thus the miscibility gap  $x \approx 0.55\text{--}0.85$ , open until now, was closed. As revealed by  $^{19}\text{F}$  MAS NMR chemical shift values for the fluorite lattice and for the F1 site in the tysonite lattice, the structure of  $\text{Ba}_{1-x}\text{La}_x\text{F}_{2+x}$  continuously changes from fluorite to tysonite in the range  $x \approx 0.70\text{--}0.85$ . Moreover, the  $^{19}\text{F}$  chemical shifts for the F2 and F3 sites in the tysonite lattice, which could not be discriminated here, tend towards those for the F1 site with decreasing  $x$ . Complete motional narrowing of the static  $^{19}\text{F}$  NMR lines of the samples with  $0.10 \leq x \leq 0.50$  at  $T \geq 453$  K indicates that the corresponding fluoride ions are highly mobile. In the samples with  $0.60 \leq x \leq 0.85$ , the number ratio of slow (or non-mobile) to highly mobile fluoride ions increases with increasing  $x$ . Furthermore, a change of the fluoride ion conduction mechanism can be observed by analyzing the shape of the NMR lines. See page 7117.

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[dx.doi.org/10.1021/jp408574d](https://doi.org/10.1021/jp408574d)

**Dynamic Effects on the Charge Transport in an Organic Near-Infrared Absorber Material**

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[dx.doi.org/10.1021/jp411152s](https://doi.org/10.1021/jp411152s)

**Direct Observation of Active Material Concentration Gradients and Crystallinity Breakdown in  $\text{LiFePO}_4$  Electrodes During Charge/Discharge Cycling of Lithium Batteries**

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[dx.doi.org/10.1021/jp411285z](https://doi.org/10.1021/jp411285z)

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Jhimli Sarkar Manna,\* Debmallya Das, and Manoj K Mitra

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[dx.doi.org/10.1021/jp4114199](https://doi.org/10.1021/jp4114199)

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[dx.doi.org/10.1021/jp4127573](https://doi.org/10.1021/jp4127573)**Reassembly and Oxidation of a Silver Nanoparticle Bilayer Probed by in Situ X-ray Reciprocal Space Mapping**

Peter Siffalovic,\* Karol Vegso, Monika Benkovicova, Matej Jergel, Andrej Vojtko, Martin Hodas, Stefan Luby, Hsin-Yi Lee, Ching-Shun Ku, Man-Ling Lin, U-Ser Jeng, Chun-Jen Su, and Eva Majkova

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[dx.doi.org/10.1021/jp412802h](https://doi.org/10.1021/jp412802h)**Portable Visible-Light Photocatalysts Constructed from Cu<sub>2</sub>O Nanoparticles and Graphene Oxide in Cellulose Matrix**

Kai Tu, Qiyang Wang, Ang Lu,\* and Lina Zhang\*

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[dx.doi.org/10.1021/jp500453v](https://doi.org/10.1021/jp500453v)**Pu@C<sub>24</sub>: A New Example Satisfying the 32-Electron Principle**

Debashree Manna, Abhishek Sirohiwal, and Tapan K. Ghanty\*

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[dx.doi.org/10.1021/jp500528n](https://doi.org/10.1021/jp500528n)**Thermal Sensitive Quantum and Phonon Confinements for Temperature Mapping in Extreme Environments**

Ashish Kumar Mishra, Junwei Wang, and Liping Huang\*

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[dx.doi.org/10.1021/jp501122n](https://doi.org/10.1021/jp501122n)**Conductance of Well-Defined Porphyrin Self-Assembled Molecular Wires up to 14 nm in Length**

Quirina Ferreira,\* Ana M. Bragança, Luís Alcácer, and Jorge Morgado

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[dx.doi.org/10.1021/jp501613b](https://doi.org/10.1021/jp501613b)**DNA-Mediated Anomalous Optical Coupling of Heterogeneous Metallic Nanostructures**

Shiho Tokonami,\* Keisuke Nishida, Shimpei Hidaka, Yojiro Yamamoto, Hidenobu Nakao, and Takuya Iida\*

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[dx.doi.org/10.1021/jp501734s](https://doi.org/10.1021/jp501734s)**Tuning Electronic and Magnetic Properties of Early Transition-Metal Dichalcogenides via Tensile Strain**

Hongyan Guo, Ning Lu, Lu Wang, Xiaojun Wu,\* and Xiao Cheng Zeng\*

## Additions and Corrections

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[dx.doi.org/10.1021/jp502302y](https://doi.org/10.1021/jp502302y)**Correction to "Synthesis, Structure, and Luminescence Properties of K<sub>2</sub>Ba<sub>7</sub>Si<sub>16</sub>O<sub>46</sub>:Eu<sup>2+</sup> for White Light Emitting Diodes"**

Wenzhen Lv, Yongchao Jia, Qi Zhao, Wei Lü, Mengmeng Jiao, Baiqi Shao, and Hongpeng You\*

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