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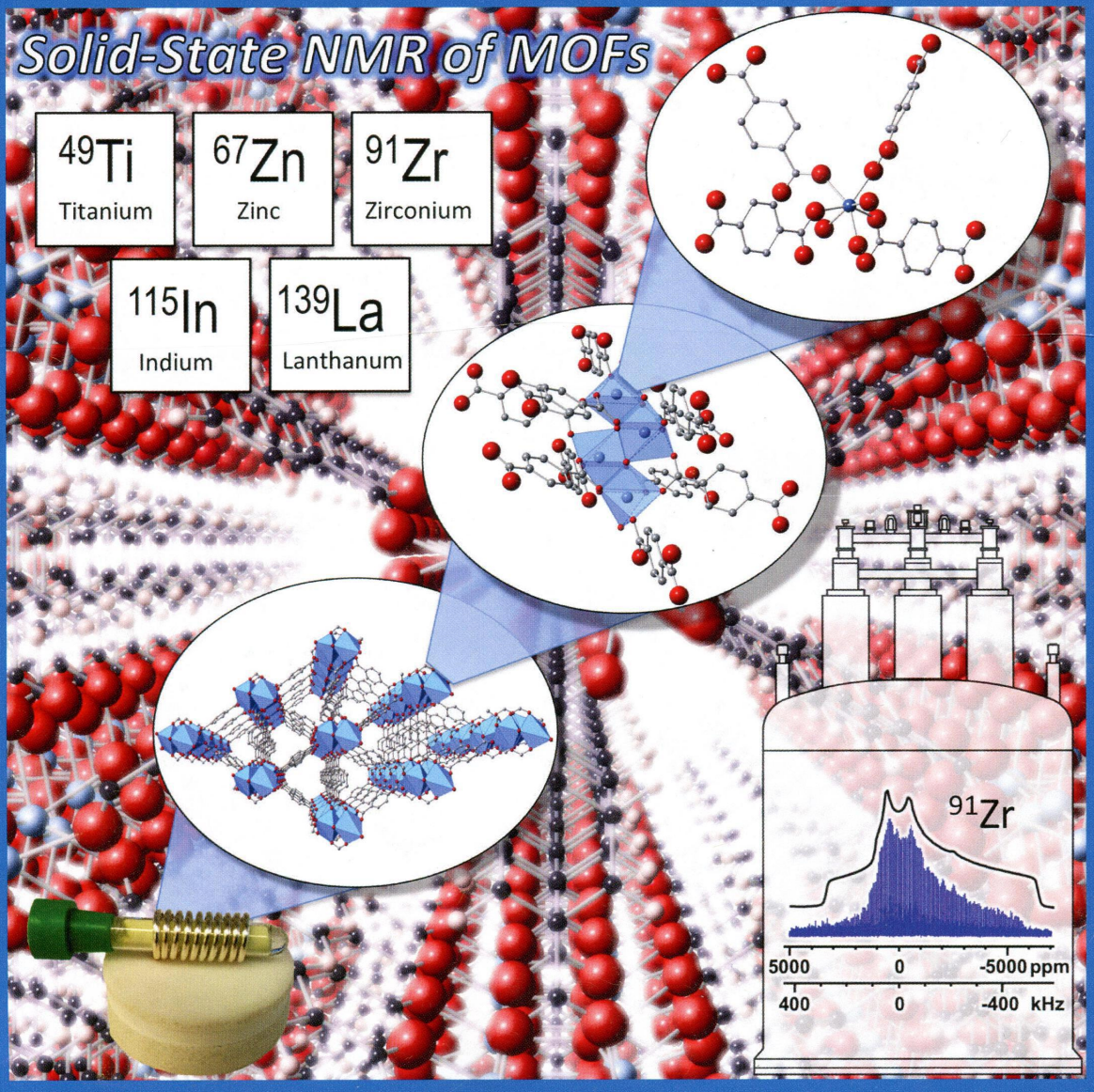

Solid-State NMR: Yielding Rich Information on Local Environments of Metals within Metal-Organic Frameworks (see page 23728)

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

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ON THE COVER: Solid-state NMR: yielding rich information on local environments of metals within metal-organic frameworks. Solid-state NMR spectroscopy (SSNMR) targeting NMR-active metal centers at natural abundance, in concert with ab initio density functional theory calculations and X-ray diffraction, is a powerful tool for elucidating the molecular-level structure of metal-organic frameworks (MOFs). ^{91}Zr, ^{115}In, ^{139}La, $^{47/49}$Ti, and ^{67}Zn SSNMR experiments are sensitive to subtle differences in coordination, bond length distribution, and ligand geometry about the metal center within MOFs. SSNMR spectroscopy of metal centers offers an impressive addition to the arsenal of the techniques for MOF characterization. On the cover, the structure of the MOF MIL-140A is shown at three different magnifications, representing the detailed structural information available from SSNMR experiments. The corresponding ^{91}Zr SSNMR spectrum of MIL-140A acquired at a magnetic field of 21.1 T is shown in the bottom right. The background is a perspective view down one of the channels within the MIL-140A crystal structure. See page 23728.

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Energy Conversion and Storage; Energy and Charge Transport

23443 (S) dx.doi.org/10.1021/jp503495k

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23459 (S) dx.doi.org/10.1021/jp5047479

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23468 (S) dx.doi.org/10.1021/jp5048562

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23476 (S) dx.doi.org/10.1021/jp505957q

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23701 dx.doi.org/10.1021/jp505490c

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Comments

24197 dx.doi.org/10.1021/jp505703k
Comment on "Breakdown of Exciton Splitting through Electron Donor−Acceptor Interaction: A Caveat for the Application of Exciton Chirality Method in Macromolecules"
Gennaro Pescitelli* and Lorenzo Di Bari

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