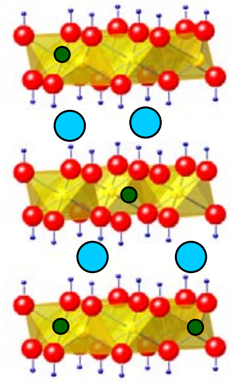
Positively Made to Order

900-MHz NMR studies are a step toward tailored anion exchangers



LDHs consist of hydroxide sheets containing cations (green and yellow) separated by anions (blue) and structural water molecules.

Studies using EMSL's 900-MHz nuclear magnetic resonance spectrometer are proving to be a solid stepping stone towards made-to-order materials for catalysis, drug delivery, and environmental remediation. Researchers from Stony Brook University used EMSL's high-field NMR spectrometer to study an unusual and versatile family of materials—layered double hydroxides, or LDHs. LDHs consist of a framework of cation-containing metal hydroxide sheets separated by anions and structural water molecules. This intercalated sheet structure can accommodate a variety of cations in the sheets and anions in the interlayer, resulting in many possible material compositions and, therefore, many potential applications. LDH applications depend upon anion exchange, such that anions in the LDH interlayer are exchanged for anions in another chemical or material. For example, LDHs can be used to sequester the toxic anion, chromate, from contaminated environments.

Ultimately, the anion exchange ability and anion selectivity of LDHs are dictated by the number and arrangements of the different cations in the sheets of the structure. Therefore, to understand how to tailor LDHs for a particular application, it is first necessary to understand the cation distribution. Conventional diffraction and spectroscopy methods to characterize LDH structures have proved inadequate, so the research team turned to EMSL's 900-MHz NMR spectrometer and its customized probe technologies. The team used EMSL's ^{25}Mg magic-angle spinning NMR probe to yield high-resolution spectra for three analogs of a naturally occurring LDH, hydrocalcite. The three hydrocalcite-like LDHs studied have magnesium and aluminum occurring in different ratios, such that they contain 19%, 25%, and 33% aluminum. The low and medium aluminum-composition samples were found to have a nonrandom distribution of magnesium and aluminum cations. The sample containing 33% aluminum was found to have a highly structured honeycomb arrangement of magnesium and aluminum cations.

Scientific impact: Understanding the cation arrangements in LDHs enables new approaches to design them with desired functionality. In addition, the technique used to characterize LDHs using the ^{25}Mg magic-angle spinning NMR probe will have broad applications to similar systems of study, allowing advances in EMSL's focus to characterize surfaces and interfaces with unprecedented resolution.

Societal impact: LDHs are versatile materials that already have demonstrated capabilities for catalysis, drug delivery, and environmental remediation. The power to tailor them could lead to refined materials for established applications as well as to new materials for unexplored applications.

For more information, contact EMSL Communications Manager Mary Ann Showalter (509-371-6017).

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