Mechanosynthesis and solid-state NMR for new materials discovery

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Conventional materials synthesis is usually time consuming. How can we make new materials more rapidly? Mechanochemistry is an appealing strategy as it enables the synthesis of 10-20 new materials in a single 30-minute run without the use of solvents or the need for purification. The capacity to quickly make large and diverse libraries of materials allows us to focus on understanding them. Determining the structure-property relationships at multiple length scales is key for rational design of new materials. For example, diffraction techniques offer insight into the long-range structure of solids. However, many properties are determined by local structure, which can be accessed using approaches based on, e.g., total scattering (PDF), XAFS, and magnetic resonance (NMR and ESR).

I will use the example of metal halide perovskites, an intensely studied class of optoelectronic materials, to show how we can determine the atomic-level structure of solids in an element-specific manner using solid-state NMR. The research questions range from quantifying dopant incorporation, phase segregation, decomposition pathways, to structural dynamics.

I will then show examples from other areas of materials research where solid-state NMR has been key to understanding atomic-level processes occurring on surfaces, inside porous materials and in bulk molecular solids. I hope that sharing these ideas will stimulate a productive and inspiring discussion.