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New classes of piezoelectrics, ferroelectrics, and antiferroelectrics by first-principles high-throughput materials design

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Functional materials, such as piezoelectrics, ferroelectrics, and antiferroelectrics, exhibit large changes with applied fields and stresses. This behavior enables their incorporation into a wide variety of devices in technological fields such as energy conversion/storage and information processing/storage. Discovery of functional materials with improved performance or even new types of responses is thus not only a scientific challenge, but can have major impacts on society. In this talk I will review our efforts to uncover new families of functional materials using a combined crystallographic database/high-throughput first-principles approach. I will describe our work on the design and discovery of thousands of new functional materials, specifically the LiAlSi family as piezoelectrics, the LiGaGe family as ferroelectrics, and the MgSrSi family as antiferroelectrics.