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Magnetoelectric coupling in multiferroic materials from first principles

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The combination of magnetic and ferroelectric properties in a single material is very appealing both because of the interesting coupling effects that emerge as well as due to a variety of technological applications that can be envisaged. Computational methods based on density functional theory have made invaluable contributions to the present understanding of such magnetoelectric multiferroics. In this talk I will show how we use these methods to understand the intriguing properties of presently known multiferroics and to design new multiferroic materials with more desirable properties. In particular, I will focus on the coupling between structural distortions and so-called "weak" magnetic order that is mediated by the Dzyaloshinskii-Moriya interaction, and I will discuss the possibility of electric-field induced magnetization switching in prototypical multiferroic systems such as $BiFeO_3$ and $BaNiF_4$.