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First-principles-derived spin models for the electric control of magnetism in $BiFeO_3$ JUN HEE LEE, RANDY FISHMAN, Materials Science and Technology Division, Oak Ridge National Laboratory — While various spin models excellently describe long-range spin spiral states in complex materials, they do not capture atomistic behavior with respect to external perturbations such as electric field or strain. On the other hand, while first-principles approaches capture the atomistic behavior, they cannot practically deal with large systems with long-range spin ordering. In this talk, we demonstrate how spin models and first principles can be synergetically combined to understand the response of complex spin systems with respect to electric field or strain. We present first-principles-derived spin models that show excellent agreement with experimental spin-wave excitations driven by electric field or strain in $BiFeO_3$. With the atomistic model, we will discuss how to effectively control magnetism in $BiFeO_3$ with the combination of electric field and strain.

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