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Density Functional Theory of Multiferroics

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The electronic and structural properties of complex magnetic oxides are notoriously difficult to calculate accurately because of the strong correlations between their localized, magnetic electrons. Indeed with the traditional local density approximation to density functional theory, ferromagnetic metallic behavior is often predicted for materials which are known experimentally to be antiferromagnetic insulators. This is particularly problematic in the modeling of multiferroic materials, because such spurious metallicity is fundamentally incompatible with the occurrence of ferroelectricity. Fortunately methodological advances such as the LDA+U method, and the use of self-interaction corrections, now allow the reliable calculation of multiferroic phenomena without significant increase in computational cost. Here we review the utility of such modern density functional methods in explaining and predicting multiferroic behavior. We describe the elucidation of ferroelectric mechanisms that are compatible with magnetism, the successful prediction and subsequent synthesis of new multiferroics, and some recent computational explorations of magneto-electric switching.