Computational design of contraindicated multifunctional materials; combining magnetism with additional functionalities

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There has been tremendous recent interest in multifunctional or "smart" materials, such as piezoelectrics, magnetostrictive materials, shape memory alloys, and piezomagnets, to name a few. Such materials find widespread and diverse applications, for example in medical ultrasound devices, smart structures in automobiles, navalsonar and micromachines, however the fundamental physics behind their functionalityis often poorly understood. Of particular interest, both from a basic scientific andan applications perspective are materials that combine pairs of contraindicatedfunctionalities, such as ferromagnetism and ferroelectricity. Such "multiferroics"have a spontaneous magnetization which can be switched by an applied magnetic field,a spontaneous polarization which can be switched by an applied electric field, andoften some coupling between the two. Here we use the study of multiferroics toillustrate how modern computational and theoretical tools can provide invaluablebasic insight into functional behavior, and in turn enable the development of newdevice paradigms based on combinations of functionalities. First we determine thefundamental physics behind the scarcity of ferromagnetic ferroelectric coexistence,and show that in general the transition metal d electrons, which are essential formagnetism, reduce the tendency for off-center polar distortions. Then weidentify the chemistry behind the additional electronic or structural driving forcesthat must be present for ferromagnetism and ferroelectricity to occur simultaneously.Finally we describe the successful rational design and subsequent synthesis of somenew multiferroic materials and outline some of the many exciting avenues for furtherwork in the field.