

Novel forms of energy in ferroelectric, antiferroelectric, antiferrodistortive, magnetic and multiferroic materials

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Discovering new energy terms in materials is obviously of fundamental interest and may lead to the understanding of complex phenomena. Discovery of such terms may also help us design materials with novel or optimized properties, and thus lead to new devices and advances in technology.

The aim of this talk is to report and discuss novel energy terms that have been recently proposed to exist in a variety of materials and their fundamental and practical implications:

- (1) A rather simple energy term containing four different macroscopic terms was suggested in Ref. [1] to explain and understand coupled magnetic orders (and the directions of the simultaneously-occurring ferromagnetic and/or antiferromagnetic vectors) in terms of anti-phase and/or in-phase oxygen octahedra tiltings, in magnetic and multiferroic perovskites. This energy is derived from a suggested simple microscopic formula, and takes its root in the Dzyaloshinsky-Moriya interaction. Comparison with data available in the literature and with first-principles calculations confirms the validity of such simple energy term quite generally for any tested structural paraelectric and even ferroelectric phase, and for any chosen direction of any selected primary magnetic vector.

- (2) Two elemental interatomic couplings that control the collaborative (as opposed to competing) interaction between the O₆ octahedral rotations (usually called antiferrodistortive or AFD modes) and the antiferroelectric (AFE) displacement patterns of the A-site cations in oxides with the ABO₃ perovskite structure were identified in Ref. [2]. Straightforward analytical derivations allowed us to reproduce and explain the origin of various long-range AFE orders that have been previously found in different phases of several perovskite compounds, all possessing simple or even complex long-range

AFD patterns. Our analysis also predicts new peculiar combinations of AFD and AFE orders that are waiting to be observed. Interestingly, the generalization of these two elemental interatomic couplings to superlattices made of paraelectric perovskites is straightforward [3] and it allows not only to understand the so-called hybrid improper ferroelectricity [4-7], but also to design near room-temperature multiferroics with tunable ferromagnetic and electrical properties [8].

- (3) An novel energy involving trilinear coupling between polarization, octahedral tilting and an antiferroelectric distortion was found in Ref. [9] for some structural phases. The existence of this energy combined with that indicated in item (1) results in the emergence of a novel magnetoelectric effect that makes it possible to control magnetism with an electric field via a two-step process.

- (4) Starting from the known control of magnetic vortices by the cross-product of electric and magnetic fields [10-13], Ref. [14] demonstrated that the angular momentum density associated with an electromagnetic field can directly couple with magnetic moments to produce a physical energy. Remarkably, this new form of energy was further found to reproduce in a straightforward manner and to naturally explain many complex effects. Examples include the spin-current model in multiferroics [14], the anomalous Hall effect [15], and the anisotropic magnetoresistance and the planar Hall effect in ferromagnets [16]. This energy also led to the prediction of novel spintronic effects [17] that bear resemblance to the so-called inverse Rashba-Edelstein effect.

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