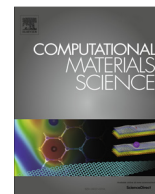




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# Theoretical studies of all-electric spintronics utilizing multiferroic and magnetoelectric materials

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## ABSTRACT

Multiferroic and magnetoelectric materials are considered as major candidates for next-generation information storage technologies due to their simultaneous presence and interplay of two or more ferroic orders. In this paper, we briefly review our theoretical progress relating to the all-electric spintronics, i.e., spin manipulation via an electric means rather than a magnetic field. Special focus is given to interface/surface magnetoelectric effect, electric field control of magnetocrystalline anisotropy, Rashba spin–orbit coupling, spin transport, and other generalized all-electric modulation of magnetism. Our recently developed method, i.e., the orbital selective external potential method, is also expounded. This method might be a powerful tool in finding the mechanisms responsible for the intriguing phenomena occurred in multiferroics or magnetoelectric materials.

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## 1. Introduction

Multiferroics are materials where two or more ferroic orders coexist owing to the interplay among spin, charge, lattice and orbital degrees of freedom. Coupling between electric and magnetic order parameters in multiferroic and magnetoelectric materials, i.e. magnetoelectric effect, provides an alternative way to control the magnetism electrically or dielectric properties magnetically. Many applications based on magnetoelectric effect have been proposed, including energy and frequency converter, transformer and gyrator, field sensor, modulator, signal amplifier, etc. [1]. However, the biggest impetus of the research on magnetoelectric effect probably comes from its potential application in the information processing industry. It therefore becomes the important topic of a new branch of spintronics, i.e. all-electric spintronics, which requires spin manipulation via electric means. Compared to the control of magnetization by the traditional magnetic field or the more advanced spin-current method, the electric approach has an apparent advantage, as it requires much lower power to switch the magnetization and might bring revolutions in the field of data storage with ultra-high speed and ultra-low power consumption.

In this review, we will briefly summarize our representative theoretical improvements in all-electric spintronics based on multiferroic and magnetoelectric materials. Starting from interface/surface magnetoelectric effect, the electric field control of magnetocrystalline anisotropy, Rashba spin–orbit coupling (SOC), and spin transport will be introduced. Other generalized electrically controlled magnetism will also be discussed. Particularly, we will describe our recently developed approach, i.e. the orbital selective external potential (OSEP) method.

Due to the lack of single-phase multiferroics combining large and robust electric and magnetic polarizations at room temperature [2], the research of all-electric spintronics mainly focus on magnetoelectric compounds by artificially fabricating ferroelectrics and ferromagnets in nanoscale heterostructures. For quite a long time, the coupling between elastic components of the ferromagnetic and ferroelectric constituents through the strain is regarded as the only source of a magnetoelectric effect in composite multiferroics. As is to be shown in details later, we explored several novel magnetoelectric effects that are significantly different from traditional ones. These studies have enriched the understanding on the interactions between electric and magnetic orders in materials, and maybe helpful to the realization of magnetic manipulation via electric ways.

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## 2. Interface magnetoelectric effect

We first describe quantum mechanical origin of the magnetoelectric effect at the interface, which opened a new route to control magnetic properties of thin-film layered structures by electric fields. In 2006, based on first-principles calculations, Duan et al. [3] found that there exists a strong magnetoelectric effect in ferromagnetic/ferroelectric multilayers, deriving from atomic bonding at the ferromagnet/ferroelectric interface. For the Fe/BaTiO<sub>3</sub>(100) heterostructure as shown in Fig. 1(a), when the BaTiO<sub>3</sub> is under the paraelectric state, the magnetic moments of the interfacial atoms are exactly the same at the bottom and top interfaces due to the structural symmetry. Note that the Fe–TiO<sub>2</sub> bonding results in sizeable induced magnetic moments in Ti atoms, which are antiparallel to the adjacent Fe atoms. When the inversion symmetry is broken by the upward polarized BaTiO<sub>3</sub>, the Ti atoms move toward the top interface and enhances the hybridization between Fe-3d and Ti-3d orbitals at the top surface (Fig. 1(b)), which increase the induced magnetic moment on top Ti atoms but reduce the magnetic moment of top Fe atoms. Since the magnetic moments are sensitive to the interfacial bonding strength, they can be controlled by the direction of ferroelectric polarization in BaTiO<sub>3</sub>. The magnetoelectric coefficient driven by interface bonding is predicted up to 0.01 G cm/V, as large as that induced by strain.

Our further study [4] revealed that the change of the interface magnetization is not the only consequence of the electric polarization reversal in such multilayers. The orbital magnetic moments and, in turn, the magnetocrystalline anisotropy energy (MAE) of Fe atoms at the interface could also be affected. As shown in Fig. 2, the magnetoelectric effect at the interface alters the MAE of a Fe monolayer by as much as 50%. With the magnetocrystalline anisotropy and the additional thickness-dependent shape anisotropy, the discovery may be helpful in writing on high coercivity perpendicular media using electric field.

Inspired by the theoretical achievements, Sahoo et al. [5] deposited a 10 nm thick Fe film on a single-crystal BaTiO<sub>3</sub>(100) substrate by molecular beam epitaxy. Up to 20% coercivity change is achieved via electrical control at room temperature. Nevertheless, the polycrystalline nature of the top Fe film reveals that the primary mechanism of the magnetoelectric effect is the interface strain coupling.

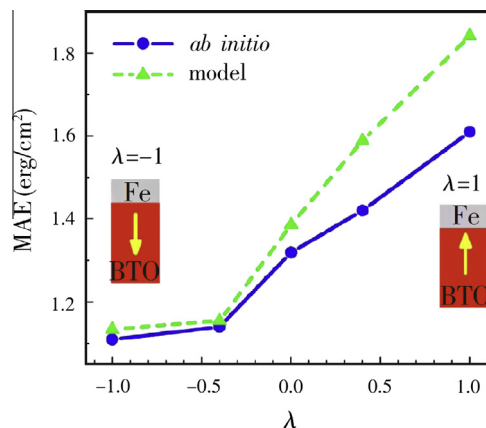


Fig. 2. MAE as a function of a polarization scaling factor  $\lambda$ . Here,  $\lambda = 1$  and  $\lambda = -1$  correspond to the spontaneous ferroelectric polarization up and down, respectively. (From Ref. [4].)

Compared with the strain-mediated magnetoelectric effect that is sensitive to the intensity instead of the direction of ferroelectric polarization, the effect driven by the ferromagnetic/ferroelectric interface bonding has the potential application in magnetic data storage without external magnetic field. In 2010, Garcia et al. [6] fabricated Fe/BaTiO<sub>3</sub>/La<sub>0.67</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> multiferroic tunnel junction and experimentally confirmed the existence of the new magnetoelectric effect. Besides the ferromagnetic/ferroelectric multilayers, the interface magnetoelectric effect has also been found in the ferromagnetic/ferroelectric Fe<sub>3</sub>O<sub>4</sub>/BaTiO<sub>3</sub>(001) interfaces [7].

## 3. Surface magnetoelectric effect

Besides the interface magnetoelectric effect in heterostructures, exploring the direct influence of an external electric field on magnetic properties of ferromagnetic metals is another important task in the research of the magnetoelectric effect.

For a ferromagnetic metal, due to the spin-dependent screening effect [8], i.e. the spin up and down electrons will have quite different responses to electric field penetrating into the ferromagnet. The spin accumulation of screening charges at the surface directly affect the surface magnetization. Since this type of magnetoelectric

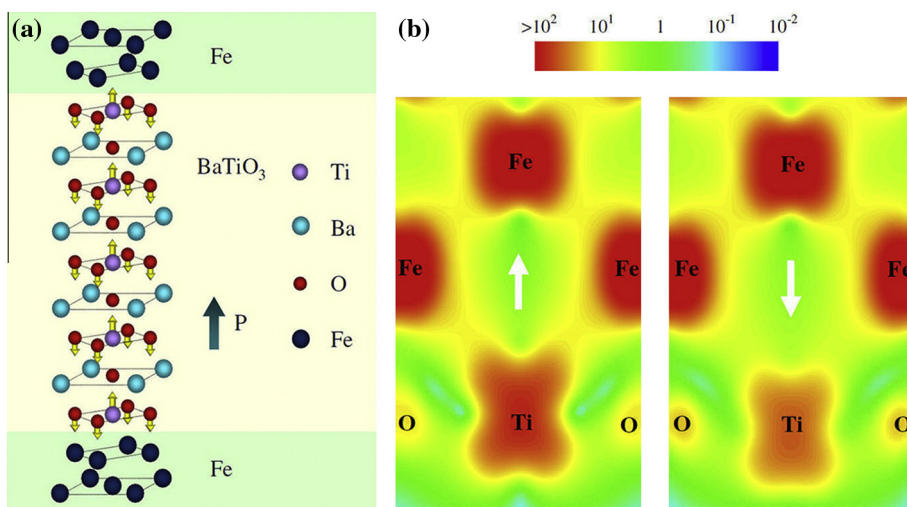


Fig. 1. (a) Atomic structure of Fe/BaTiO<sub>3</sub> multilayer for  $m = 4$ . (b) Minority-spin charge density at the Fe/BaTiO<sub>3</sub> interface for two opposite polarizations in BaTiO<sub>3</sub>. (From Ref. [3].)

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