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Theoretical studies on new mechanisms of ferroelectricity and multiferroicity

Abstract:

Ferroelectric (FE) and multiferroic (coexisting ferroelectricity and magnetism) materials have attracted numerous interest over several decades due to the exciting possibility of novel applications such as non-volatile memory. To design high-performance ferroelectrics and multiferroics, it is highly desirable to discover new mechanisms of ferroelectricity and multiferroicity. Recently, we made some progress in this direction:

(1) It is generally believed that the oxygen octahedral rotation (an AFD mode) and FE mode in ABO_3 perovskites tend to compete and suppress each other. We reveal a dual nature of the FE—AFD coupling, i.e., it turns from competitive to cooperative as the AFD mode strengthens. We provide a unified model of such a dual interaction by introducing novel high-order coupling terms, and explain the atomistic origin of the resulting new form of ferroelectricity in terms of universal steric mechanisms [1].

(2) We discover that the ferroelectricity in SnTe and perovskite oxides thin films might increase with the decrease of the film thickness, in sharp contrast to the usual trend [2,3].

(3) It was known that either charge order (CO) or orbital order (OO) can lead to ferroelectricity. In some case where the individual CO or OO cannot ensure the appearance of ferroelectricity, we find that ferroelectricity may arise due to the simultaneous presence of CO and OO. On the basis of this new mechanism, we reveal that that $(CrBr_3)_2Li$ is a 2D ferromagnetic FE multiferroic with the asymmetric Jahn-Teller distortions [4].

(4) We propose that the hydroxide may act as a new knob to simultaneously control the magnetization and polarization. This may pave a new way to realize ultimate high-density memory using a single isolated hydroxide to represent one bit [5].

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