Vibronic magnetoelectric effects in Bi-based multiferroics

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A detailed theory of electron-lattice (vibronic) covalent hybridizations [1] between the Bi 6s lone electron pair and empty oxygen 2p states which lead to ferroelectricity is presented for Bi-based multiferroics. The vibronic interactions are the driving and stabilization forces of the phase transformations in these compounds. We derived the free energy of the Bi-based multiferroics with the ferroelectric and G-type antiferromagnetic phase transitions. At this, the Zeeman splitting of electron states in an external magnetic field and the spin-phonon couplings are very important. The energy of the magnetoelectric coupling connected with the antiferromagnetism which is determined by the difference of the magnetization vectors of the sublattice of the Fe ions contributes also to the free energy. The available experimental data are analyzed using this free energy.

References:

[1] P. Konsin and B. Sorkin, Phys. Status Solidi C 6, 2759-2761 (2009).

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