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First Principles Study on Magnetoelectric Effects in $\text{Ba}_2\text{CoGe}_2\text{O}_7$

KUNIHICO YAMAUCHI, ISIR-SANKEN, Osaka University, Japan, SILVIA PICOZZI, CNR-SPIN, L'Aquila, Italy — Magnetoelectric (ME) effects, or magnetically-induced ferroelectricity, are attracting large interests due to promising applications for novel type of devices. While the microscopic origin of ME effects is mostly classified as relate to spin current and/or exchange striction, a novel mechanism originating in spin- dependent p - d hybridization has been proposed and well explained ME effects observed in antiferromagnetic $\text{Ba}_2\text{CoGe}_2\text{O}_7$. In this study, we theoretically confirmed the magnetically induced electric polarization, whose size is dependent on the direction of Co spins. By means of both Landau theory and density functional calculations, the behavior of the experimentally observed polarization was well reproduced. Microscopically, we suggest single-site spin orbit coupling to slightly change the Co- d orbital shape upon changing the direction of Co spins, resulting in “asymmetric” p - d hybridization and consequent change in the electric polarization.

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