First-principles Calculation of Electric Field Effects in Spin-to-charge Conversion Materials

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We have studied materials possessing the Rashba effect that induces spin splitting, which is applicable to spin-to-charge conversion [1]. The Rashba effect originates from spin-orbit interaction and spatial inversion symmetry breaking, and is controlled by electric fields. Based on the modern theory of electric polarization, one can apply uniform electric fields even for bulk insulators in calculations with density functional theory (DFT) codes with the periodic boundary condition [2]. We have developed a linear-combination-of-pseudo-atomic-orbital (LCPAO) version of such a function making **k**-dependent potentials and implemented it to the OpenMX code. This year, we tried to focus on electric field effects in such Rashba systems with Berry phases by using the OpenMX code. Under an electric field, cations or anions are expected to shift their positions slightly, but shifts of ions' positions induce such a large electric polarization that Rashba spin splitting occurs. During structural relaxation, such ions move by following forces on themselves, but the forces are often smaller than a usual criterion of calculated forces (e.g. 10^{-4} Ha/Bohr) when we consider the realistic strength of electric fields. However, for nonorthogonal cells such as hexagonal cells, in the case of generalized gradient approximation (GGA), the "egg box effect" appeared as a difficulty because OpenMX uses PAOs expanded in the real space grid to compute physical quantities, but description of PAOs depends on the origin of the grid, that is, introducing the grid causes numerical errors. To overcome the difficulty, we added functions of calculations of a total energy and forces with several grid origins. Once calculations of electronic systems converge, one can get density matrices (DMs) and taking another real space grid with a different origin, one can evaluate an energy and forces again with the frozen DMs. In the way, we succeeded in evaluating forces under electric fields with a moderate number of grids (i.e. cutoff energy). We also added a function to change the order of the Lagrange interpolation to estimate density gradients, and it improved evaluation of forces. These two functions enabled us to predict not only relaxed structures under electric fields but also static dielectric constants and Born effective charges in any cell shape. Indeed, we confirmed that our calculated values of dielectric constants and Born effective charges for typical insulators are consistent with the prior theoretical and experimental studies. Since we encountered the problems of the "egg box effect", we have not done calculations of applications, but we have suggested a simple model of surface alloys, such as Bi/Ag surface alloys inducing giant spin splitting, based on DFT calculations [3]. This year, we also succeeded in reducing half of computational time for Berry phases averagely through tuning, and running our implemented code with up to 32^3 **k**-points for zinc blende primitive cells through efficient transfer of arrays of **k**-dependent potentials in the message passing interface (MPI).

References

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