Development of First-principles Codes for Evaluation of Physical Properties Through Local Berry Phases

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This year we continued to develop the calculation code for the coefficients of the magnetic thermoelectric effects, the anomalous Hall and Nernst effects [1], as a code for the evaluation of the physical properties of the local Berry phase method. First, we performed applied calculations on the subject of Heusler alloy systems to investigate their defect effects. When expanding the system using supercells, the computational cost increases due to the larger number of atoms, but in addition, there is the problem of increasing the number of degenerate points that induce numerical instability due to the folding of the Brillouin zone. To avoid that numerical instability, we tried devising various calculation methods for the Berry curvature evaluation routine and found that the most robust results were obtained by approximating with the minor determinant. The implementation is already MPI parallelized for k points. It will also be extended to a combined version of the modified tetrahedron method, and the improved calculation code will be evaluated through trial application calculations in the future.

We have also developed a calculation method to decompose the anomalous Hall and Nernst conductivity into the contributions of each layer in layered materials. By unitary transformation of the Bloch wavefunctions, we constructed hybrid Wannier functions localized only in the direction orthogonal to the plane of each layer, formulated a method for finding the anomalous Hall conductivity at the Wannier center, and implemented the code with the MPI parallelization for the k-points. Using this, it was confirmed that the even-layered antiferromagnetic $MnBi_2Te_4$ is an axion insulator exhibiting a surface anomalous Hall effect, where the conductivity is $1/2$ in e^2/h units at the surface. The computational model was based on the structure of odd-layered $MnBi_2Te_4$ used in last year's study [2], which was an interlayer antiferromagnetic magnetic structure. Such a calculation method for "layer anomalous Hall conductivity" is expected to be applied to a wide range of systems, including two-dimensional stacking materials and artificial superlattices.

As an application of the code developed last year for the evaluation of magnetic thermoelectric properties [1], we predicted the anomalous Nernst coefficient in Cr-doped Bi_2Se_3 which is a Chern insulator [3]. The code was also used in a theoretical study of the mechanism of the giant magnetic thermoelectric effect induced by the van Hove singularities [4].

Furthermore, in the case of tight-binding models or atomic basis set, we developed a method to avoid many eigenvalue problems by combining a highly efficient Berry phase calculation routine developed last year when implementing the electric field application method [5] with the density matrix based on that basis.

The development of the above calculation codes was done while implementing them in the first-principles calculation code OpenMX [6].

References

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