**Magnetic Dipole-dipole Energy Evaluation on 1D, 2D, and 3D Periodicities using Density Functional Approach**

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Magnetic dipole-dipole interaction is one important factor for determining the magnetization direction of magnets as well as the spin-orbit interaction. Furthermore, it may also contribute to emergences of peculiar non-collinear magnetism, such as magnetic skyrmions, multi-ferroic polarization, etc. In general, the magnetic dipole-dipole interaction is estimated by the arrangement of atomic magnetic moments so far. However, in the case where there is a large spatial anisotropy in the electron spin density, reliability of that treatment remains uncertain. Therefore, we have investigated the way of estimating magnetic dipole-dipole energy through the spin density obtained from density functional theory [1,2,3].

Since the magnetic dipole-dipole interaction proportional to the minus third power of the distance between the dipoles, the effect from long distances cannot be ignored. Moreover, its long-range feature requires some special treatment for numerical evaluation, based on the dimension of periodicity and boundary condition in the target system. One can estimate the magnetic dipole-dipole energy on each dimension with a high efficiency, using the Coulomb Green function of the respective dimension (one-, two-, or three-dimension).

As a demonstration of our implementation, we calculated the magnetic anisotropy energy of simple 1D, 2D, and 3D magnetic structures. The result provided the same value as in the calculation with a localized spin moment model, assuming a spherical local spin density on each atom. Apart from this, we investigated several extreme cases for checking the implementation and reproduced the previous results successfully. In addition, we investigated magnetic anisotropy of the solid oxygen which is known as antiferromagnetic molecular crystal. In the oxygen molecule, the spin density distribution much deviates from a spherical one because of electron orbital anisotropy. We found that the spin density distribution also plays an important role for the magnetic dipole-dipole interaction aside from those of atomic spin alignment. Our results are in a good agreement with the experimental data, indicating a reliability of our method. For example, in the *α*-phase of solid oxygen, both the spin density distribution and spin-orbit interaction on molecule favor a direction perpendicular to the molecular axis and the crystal field originating from the magnetic dipole-dipole interaction limits the stable direction to the *b*-axis which has the mirror planes of the crystal structure.

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