First-Principles Study of Magnetocrystalline Anisotropy in Antiferromagnetic Fe_2As

Kisung Kang, Kexin Yang, David G. Cahill, André Schleife

When tetragonal antiferromagnetic materials have easy-plane magnetism and metallic electronic band structure, they can be a great candidate for future magnetic memory. This is because easy-plane magnetism allows storing binary information using a 90-degree in-plane switching of the Néel vector orientation. The key parameter for comprehending the switching mechanism is the magnetocrystalline anisotropy energy, which plays the role of an energy barrier between two degenerate states. In this work, we use density functional theory (DFT) and a classical magnetic dipole-dipole interaction (MDD) model to obtain the magnetocrystalline anisotropy of metallic tetragonal antiferromagnetic Fe2As. The result confirms the four-fold symmetry of in-plane anisotropy and the K_{22} coefficient of 276.5 J/m^3, which purely comes from spin-orbit interaction (SOI). It is comparable to the measured 150 J/m^3 from torque magnetometry. For out-of-plane anisotropy, the MDD becomes non-negligible due to the chemical and magnetic structure. Total out-of-plane anisotropy leads to two-fold symmetry and a K_1 coefficient of 830 kJ/m^3, with one-third due to MDD and the two thirds due to SOI. The lowest frequency of an antiferromagnetic spin-wave is predicted to be 0.64 THz, indicating fast dynamics for data storage and potential adversity of low thermal stability.

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