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Origin of huge coercivity in iron oxide ε-Fe_2O_3

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Abstract

ε-Fe_2O_3, which is a rare phase of iron oxide Fe_2O_3, was first obtained as a pure phase by our research group in 2004. It exhibits a huge coercive field of 20 kOe at room temperature, and due to the strong magnetic anisotropy, this material shows millimeter wave absorption at a very high frequency of 182 GHz.[1] In this work, we report the theoretical studies on the electronic structures of ε-Fe_2O_3 to understand its huge coercivity. Synthesis of ε-Fe_2O_3 nanoparticles uses a combination technique of reverse-micelle and sol-gel techniques. The crystal structure is orthorhombic with four different Fe sites, A, B, C, and D sites, where A, and B sites are distorted octahedral, C site is a regular octahedral, and D site is a tetrahedral site. Using this crystal structure, we studied the electronic structure using first-principles calculations and molecular orbital calculations to understand the origin of the huge coercive field.[2] The density of states showed that ε-Fe_2O_3 is a charge-transfer type insulator with positive sublattice magnetizations at B and C sites and negative sublattice magnetizations at A and D sites, consistent with our previous study based on molecular field theory.[3] The charge density map showed a strong hybridization between Fe3*d* and O2*p* orbitals. Molecular orbital calculations indicated that this hybridization originates from the distorted coordination geometry of the Fe sites. This hybridization induces charge-transfer from O2*p* to Fe3*d*, which is assumed to create a non-zero orbital angular momentum, affecting the magnetic anisotropy of ε-Fe_2O_3.

Biography

Marie Yoshikiyo has completed her bachelor and masters from Department of Chemistry, School of Science, The University of Tokyo. She is now a PhD student at The University of Tokyo under the supervision of Prof. Shin-ichi Ohkoshi. (2013-present: JSPS Research Fellowship for Young Scientists)