Marie Yoshikiyo et al., Chem Sci J 2016, 7:2(Suppl)
http://dx.doi.org/10.4172/2150-3494.C1.002

First-principles calculation of ε-Fe_2O_3 with a huge coercive field

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Iron oxide materials have contributed to our society due to their chemical stability and economical cost, for example, α-Fe_2O_3 as pigment and γ-Fe_2O_3 as magnetic recording material. In 2004, our research group succeeded in synthesizing a pure phase of a different Fe_2O_3, ε-Fe_2O_3, which exhibits a huge coercive field of 20 kOe at room temperature.1 Originating from its strong magnetic anisotropy, ε-Fe_2O_3 also shows electromagnetic wave absorption at a very high frequency of 182 GHz. In this work, we report the theoretical studies on the physical properties of ε-Fe2O3 by first-principles calculation.

ε-Fe_2O_3 has an orthorhombic crystal structure with four nonequivalent Fe sites, A, B, C, and D sites. Based on this crystal structure, we studied the electronic structure by 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 of the Fe3*d* band showed a strong hybridization with O2*p* orbitals. Molecular orbital calculations indicated that this hybridization originates from the distorted coordination geometry of the Fe sites. Due to the hybridization, charge-transfer occurs from O2*p* to Fe3*d* generating a non-zero orbital angular momentum, enhancing the magnetic anisotropy of ε-Fe_2O_3. Furthermore, electric polarization of ε-Fe_2O_3 was also investigated by first-principles calculation.

Biography

Marie Yoshikiyo received her M.Sc. in Chemistry from the University of Tokyo in 2013, and pursuing her Ph.D. under the supervision of Prof. Shin-ichi Ohkoshi. She is currently a Project Assistant Professor of Department of Chemistry, School of Science at the University of Tokyo. Her research interests focuses on the development of functional materials, especially magnetic nanomaterials based on iron oxides.

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