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## Theoretical calculations of the electronic structure and phonon modes of ε-$Fe_2O_3$ nanomagnets

ε-$Fe_2O_3$ nanomagnet, one of the four polymorphs of iron oxide $Fe_2O_3$, was first discovered by our group as a pure phase via a chemical nanoparticle synthesis, a combination of reverse-micelle and sol-gel methods. This material exhibits a large coercive field over 20 kOe at room temperature and the magnetic properties could be widely controlled by metal substitution. In this work, we report the theoretical calculations of the electronic structure and phonon modes of ε-$Fe_2O_3$.

Using the crystal structure determined by powder X-ray diffraction, we calculated the electronic structure of ε-$Fe_2O_3$ using first-principles calculations and molecular orbital calculations, and the origin of the huge coercive field was investigated. Furthermore, we calculated the phonon modes of ε-$Fe_2O_3$ using the Phonon code. The lowest vibration mode was calculated to be 2.51 THz due to the Fe atom vibration along the crystallographic a-axis with A1 symmetry. The phonon modes were experimentally observed by Far-IR spectroscopy, which showed good agreement with the calculation results. Phonon modes of metal-substituted ε-$Fe_2O_3$ are also introduced.

### Speaker 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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