Magnetism in Rutile-Type Oxides

Purev Taivansaikhan and Dorj Odkhuu^{*}
Department of Physics, Incheon National University, Incheon 22012, Republic of Korea

While rutile-type transition metal oxides (TMO₂) have been widely used in a variety of important applications such as an active catalyst, supercapacitors, batteries, and fuel cells, an existence of intrinsic magnetism in RuO₂ has recently drawn much attention in spintronics. In this talk, we will present results of our first-principles density functional theory plus U (DFT+U) calculations on magnetism and magnetic anisotropy energies (MAE) of RuO₂ and OsO₂. These oxides are identified to favor an antiferromagnetic phase, which is a result of mutual mechanisms of Kramer-Anderson superexchange interaction and Jahn-Teller effects. More remarkably, we found very large MAE up to an order of 10 meV per transition metal atom in bulk, which are four orders of magnitude greater than those of the conventional transition metals. This anisotropic phenomenon further exhibits a persistently increasing dependence of film thickness, which is very uncommon in thin film materials.