# Magnetocrystalline anisotropy in doped nickel oxides

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There has been a rapid rise in interest of antiferromagnetic materials (AFMs) in technological applications, especially, optoelectronics in a terahertz range [1] for which the key ingredient to improve the efficiency is a tuning of the magnetocrystalline anisotropy (MCA) in AFMs. Despite its importance, the MCA in AFMs, in contrast to that in ferromagnetic materials, is not well understood. Here, we carried out first principles calculations of the MCA energy in doped NiO by using the full-potential linearized augmented plane wave method [2] based on generalized gradient approximation, and discussed the dopant dependence to the MCA. The electron correlation effect at Ni sites was treated in the DFT+U scheme with an effective on-site Coulomb interaction parameter $U_{\mathrm{eff}}$ [3]. The MCA energy was obtained by the difference in total energies with the spin orbit coupling, by using force theorem,[2] for the magnetization oriented along [001], [110], and [111] doections. In the non-doped NiO, i.e., the pure NiO, the magnetic easy and hard axes result in [001] and [111] directions, respectively, which agrees with experiments. By doping 3*d* elements like Mn, however, the MCA is found to change significantly compared to that of the non-doped NiO. We have further expanded our investigation including the *sp* elements systematically. More details including mechanism of the doping effects to the MCA will be discussed.

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