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Strain effects in spinel ferrite thin films from density functional theory calculations CLAUDE EDERER, DANIEL FRITSCH, School of Physics, Trinity College Dublin, Ireland — Spinel ferrites $CoFe_2O_4$ (CFO) and $NiFe_2O_4$ (NFO) are insulating magnetic oxides with high magnetic ordering temperatures and large saturation magnetization which are of interest for spintronics applications and as building blocks of multiferroic heterostructures [1]. In both cases, strain-induced changes of the magnetic properties are particularly important. Here we present results of density functional theory calculations for the structural and magnetic properties of strained bulk CFO and NFO, with special emphasis on strain-induced changes in the magneto-crystalline anisotropy energy (MAE). Our results are representative for (001)-oriented thin films of CFO and NFO, grown on different lattice-mismatched substrates. We find a large and strongly strain-dependent MAE for CFO, and a significantly smaller but also strongly strain-dependent MAE for NFO. We discuss the influence of cation order within the inverse spinel structure and analyze the effect of different exchange correlation functionals on the structural and magnetic properties. [1] H. Zheng et al., Science 303, 661 (2004).

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