**First-principles Investigation on Al Doping in SrTiO3**

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SrTiO3 (STO) is regarded as a representative high-k material in oxide electronics, owing to its high mobility and dielectric constant (~300). However, because of its n-type nature and relatively small band gap (3.3 eV), Schottky barrier between the metal-STO interface is under 1 eV, which leads to large leakage current.

It has been repeatedly reported that the intrinsic n-type nature of STO originates from thermodynamically stable oxygen vacancy. The most straight forward approach to control the Fermi level of STO is the acceptor doping, which reduces the n-type carrier concentration and hence increases the Schottky barrier.

There have been many studies about the effect of extrinsic dopant on STO, and it was found that the doping of Feor Cr ions at Ti sites reduces the leakage current significantly. Even though it is expected that Al doping on STO should give similar behavior, the detailed analysis with regard to the doping effect has been hardly carried out.

In this study, first-principles calculation on Al dopant in STO is carried out. The defect formation energies including intrinsic defects are calculated with hybrid density functional method. The concentration of each defect configuration and the position of the Fermi level is found. This study will give a meaningful insight into the designing of oxide electronic devices.