Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A first principles study of interstitial transition metals in the SrTiO3 bulk and at the surface[1] STEVEN HEPPLESTONE, PETER SUSHKO, University College London — Recent advances in oxide thin film deposition and growth have given a new momentum to the field of oxide electronics. For example, it was found that La-doped $SrTiO_3$ shows high charge carrier mobilities and conductivity was observed near the interface with $LaAlO_3$. However, forming low-resistance Ohmic metal/oxide constants has proven to be a challenge. Recently, the interface formed by a Cr film grown on $SrTiO_3$ (001) surface has been shown to have such properties. This raises the question of whether Cr or another metal provides the lowest resistance possible. To this end, we perform ab initio calculations using the VASP package and the PBE and PBE+U functionals and examine the electronic properties of interstitial transition metal atoms (M) in the bulk $SrTiO_3$ and near $SrTiO_3$ (001) surface. We show that for surface doping, the variation in the formation energy linearly depends on the number of d-electrons in the valence shell of the M atoms. This contrasts with the formation energies of M atoms in the bulk $SrTiO_3$, where no such trend is observed and, instead, the formation energy depends on the occupancy of the e_g and t_{2g} sub-bands.

[1]EPSRC grant EP/I009973/1

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Date submitted: 14 Nov 2013 Electronic form version 1.4