Interstitial impurity-induced surface magnetism in a layered oxide surface

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We investigated the possibility of employing the polycrystalline αPbO as a spintronics device by first principles calculations based on the density functional theory (DFT). In particular, we explored the effects of 3d transition metal atom, Fe on the structural and electronic properties of the layered αPbO (001) surface. It has been proven that ferromagnetic signals in experiments are often detected in thin films[1]. We used a 2x2, 3-layered surface slab model of αPbO with 20 Å of vacuum space to simulate this environment in this study. We placed the impurity atoms in between the surface and subsurface of the crystal. The results show that the interstitial Fe interstitial forms shorter bonds with the O atoms located at the surface and second layers. Also, this impurity is found to induce magnetism in the host crystal with magnetic moment value of 2.25 μB, which is highly localised on the transition metal. In the bonding process, the Fe's lower energy lying *3d* states form overlaps with nearest neighbour O atoms with non-bonding *3d* states situated near or at the Fermi level and are spin split. These spin split orbitals induce spin polarisation of impurity states of O atoms in the subsurface. Moreover, the magnetic order is determined using the energy difference between the antiferromagnetic and ferromagnetic states. The energy difference is 0.068 eV, suggesting that Fe interstitial impurities induce ferromagnetism in αPbO [2]. In this workshop, the effects of charge carriers to the magnetic properties will be briefly discussed. Finally, the position of the Fermi level in the projected density of states (PDOS) suggests that the Zener's ferromagnetic double exchange mechanism stabilises the ferromagnetic state.

References:

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