Ab initio study of magnesium surface oxidation

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We have performed ab initio study of magnesium surface oxidation based on density functional theory methods [1] in general gradient approximation (GGA) level with Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [2]. Numerical calculations have been done with CRYSTAL14 program package [3] exploring modified Gaussian-type DZVP basis sets for magnesium and oxygen atoms from article [4]. Using super-cell approach we found magnesium surface energies to be in the range of 39 – 64 meV/ $Å^2$ for different crystallographic planes with Miller's indices (001), (100) and (110). The electron work functions found to be in the range 2.40-2.75 eV that is a little smaller of experimental value for (001) plane – 3.84 eV [5]. As we hope, the difference should be vanished after inclusion of ghost atom layer in the modeling super-cell. We have obtained good agreement with experimental data for calculated inter-layer distances for first three layers near the surface. Obtained values of oxygen adsorption energies per oxygen atom are in a good agreement with previous study with VASP program package [6], 4.9-5.1 eV. It was shown that energy profile of oxygen atom along the line perpendicular magnesium surface (001) has series of peaks which values are 0.5-1.0 eV. We have found that energy shifts of 2p electron in magnesium atoms near the surface are in the range 0.1-1.0 eV depending on oxygen density.

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