Abstract Submitted
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Sulfur adatom adsorption on α-Fe_2O_3 (0001) film studied by DFT+U method[1] JIAO AN, PRABATH WANAGURU, The University of Texas at Arlington, CONGXIN XIA, Henan Normal University, MENG TAO, Arizona State University, QIMING ZHANG, The University of Texas at Arlington — The geometric and electronic properties of a sulfur (S) atom adsorption on the hematite α-Fe_2O_3 (0001) film with have been investigated systematically by calculations based on the density functional theory. The most stable hematite α-Fe_2O_3 (0001) film with an anti-ferromagnetic arrangement is identified. The S adatom prefers to bond with three O atoms, in the center of a triangle formed by the three O atoms. The S acts as a cation at this site. The sulfur adsorption has introduced two gap states, in addition to the unoccupied surface states. Furthermore, with the most stable S-adsorption configuration, the diffusion of the S adatom from the surface to the inside is searched and the transition state along the minimum-energy pathway is also identified. The isovalent doping of S inside of the film has also been studied.

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