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First-principles studies of S-doping and adsorption with hematite α-Fe_2O_3 (0001) film[1] JIAO AN, PRABATH WANAGURU, QIMING ZHANG, University of Texas at Arlington — Based on spin-polarized density functional theory, we have investigated the atomic, electronic, and magnetic structures of hematite α-Fe_2O_3 (0001) film. An S atom adsorption on the surface of the film has then been studied. The preferred site on the surface has been identified. The changes of the electronic structure of the film have been analyzed when an O atom is substituted by an S atom at different locations inside the film. The change with the concentration of S-doping will also be discussed.

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