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Density functional theory study of the adsorption of elemental mercury on a 1T-MoS_2 monolayer

Key words: 1T-MoS_2 monolayer; Mercury capture; Adsorption mechanism; Density functional theory (DFT)

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Introduction

Elemental mercury has become a global concern because of its significant impact on human health and the ecosystem. A lot of effort has been put towards the removal of elemental mercury from the 2H-MoS_2 (prismatic structure of MoS_2). However, the mechanism of 1T-MoS_2 (polytype structure of MoS2) in Hg^0 capture remains unexplored. In this study, density functional theory (DFT) was adopted to investigate the adsorption mechanism of Hg on a 1T-MoS_2 monolayer. The different possible adsorption positions on the 1T-MoS_2 were examined.

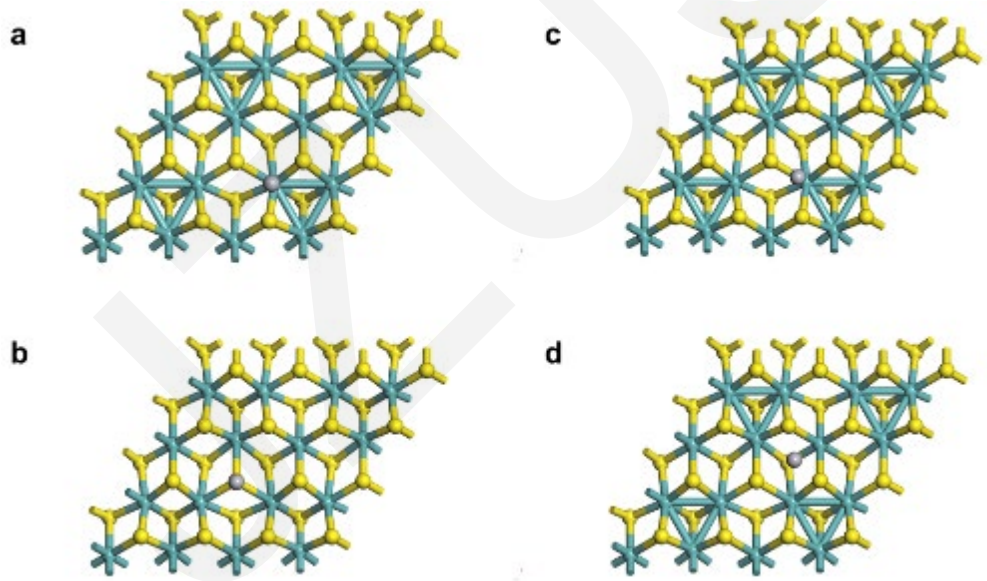
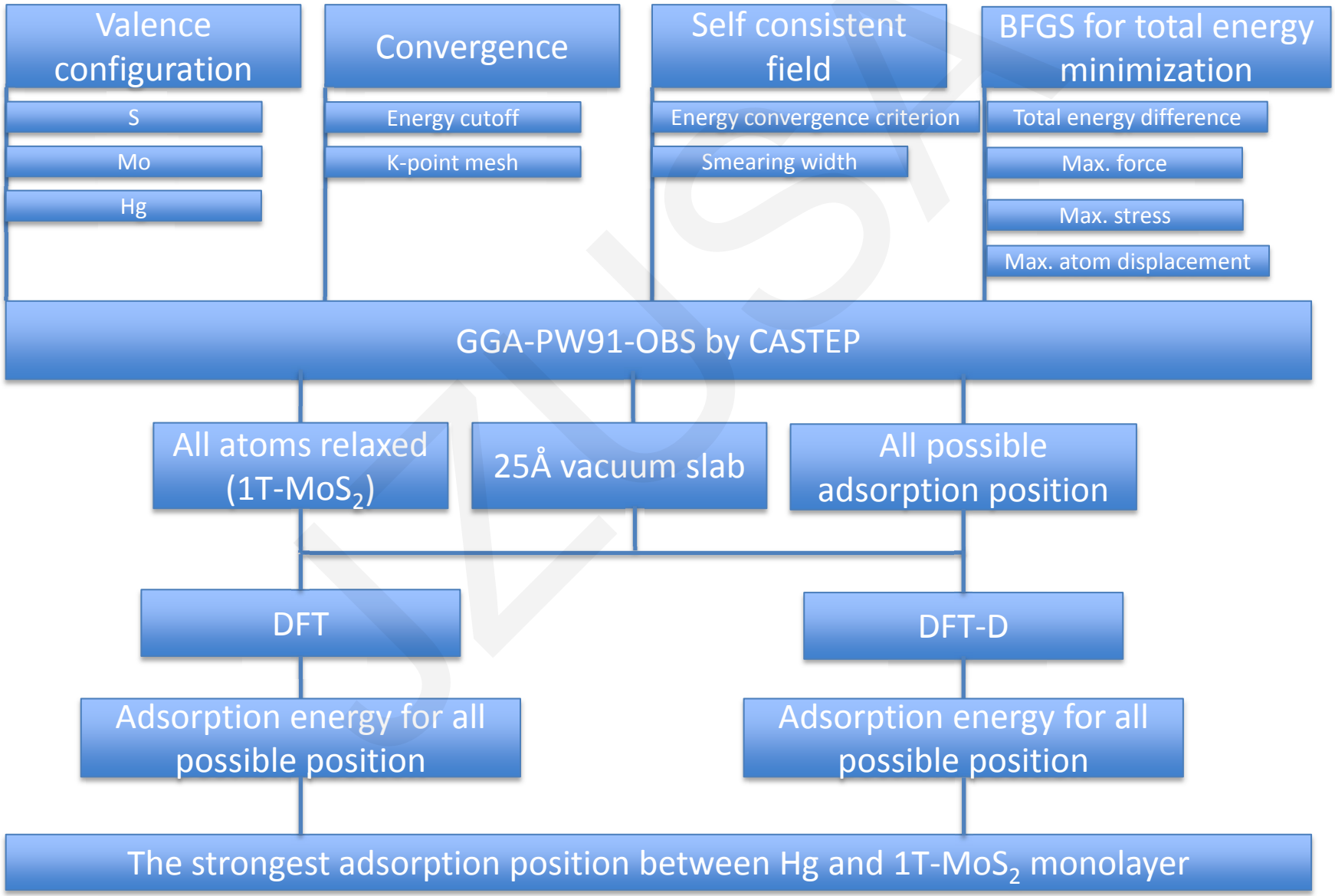


Fig. 1. Optimized stable structure of 1T-MoS_2 monolayer with adsorbed Hg atom. a. Hg atom adsorbed on the top site of a Mo atom (T_{Mo}). b. Hg atom adsorbed on the top site of the bridge site between a S-Mo bond (B_{Mo-S}). c. Hg atom adsorbed on the top site of a S atom in top Sulphur plane (TT_S). d. Hg atom adsorbed on the top site of a S atom in bottom Sulphur plane (TB_S) (yellow atom is S atom, aquamarine atom is Mo atom).

Methodology



Results and Conclusions

The results elucidate that chemisorption dominates the adsorption between Hg^0 atoms and the 1T-MoS_2. It was found that the T_{Mo} (on top of the Mo atom) position is the strongest adsorption configuration among all the possible adsorption positions. The adsorption of Hg atoms on the 1T-MoS_2 monolayer is influenced by adjacent S and Mo atoms. The adsorbate Hg^0 atom is found being oxidized on the T_{Mo} position of the 1T-MoS_2 with an adsorption energy (DFT-D)of 1.091 eV. From the partial density of states (PDOS) analysis of the atoms, the strong interaction between Hg^0 and the 1T-MoS_2 surface is caused by the significant overlap among the d orbitals of the mercury atom and the p orbitals of the S atom and p and d orbitals of the Mo atom.

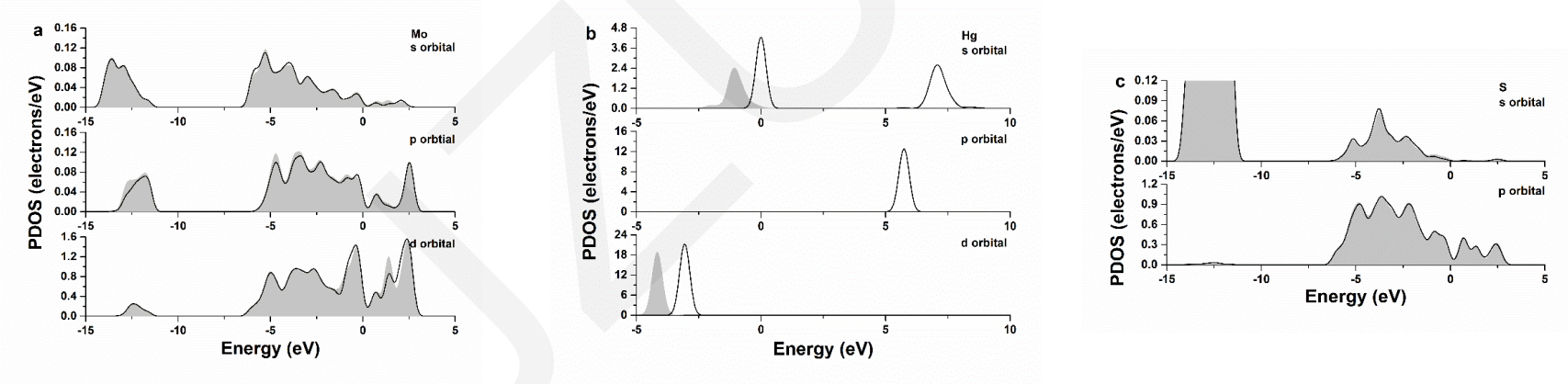


Fig.2. PDOS analysis for Hg atom and adjacent Mo and S atoms on T_{Mo} position of 1T-MoS_2 monolayer. (a) PDOS of s, p and d orbital for Mo atom. (b) PDOS of s, p and d orbital for isolated Hg atom. (c) PDOS of s and p orbital for S atom. (Black line means before adsorption, the grey shadow means after adsorption).