

**Cite this as:** Xue-liang Mu, Xiang Gao, Hai-tao Zhao, Michael George, Tao Wu, 2018. Density functional theory study of the adsorption of elemental mercury on a 1T-MoS<sub>2</sub> monolayer. *Journal of Zhejiang University-SCIENCE A (Applied Physics & Engineering)*, 19(1):60-67.

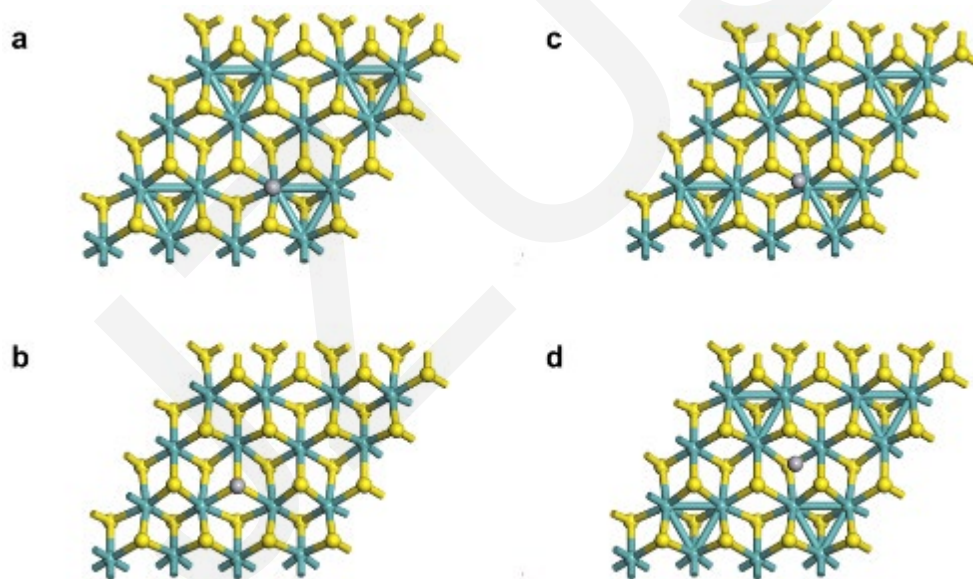
<https://doi.org/10.1631/jzus.A1700079>

## Density functional theory study of the adsorption of elemental mercury on a 1T-MoS<sub>2</sub> monolayer

**Key words:** 1T-MoS<sub>2</sub> monolayer; Mercury capture; Adsorption mechanism; Density functional theory (DFT)

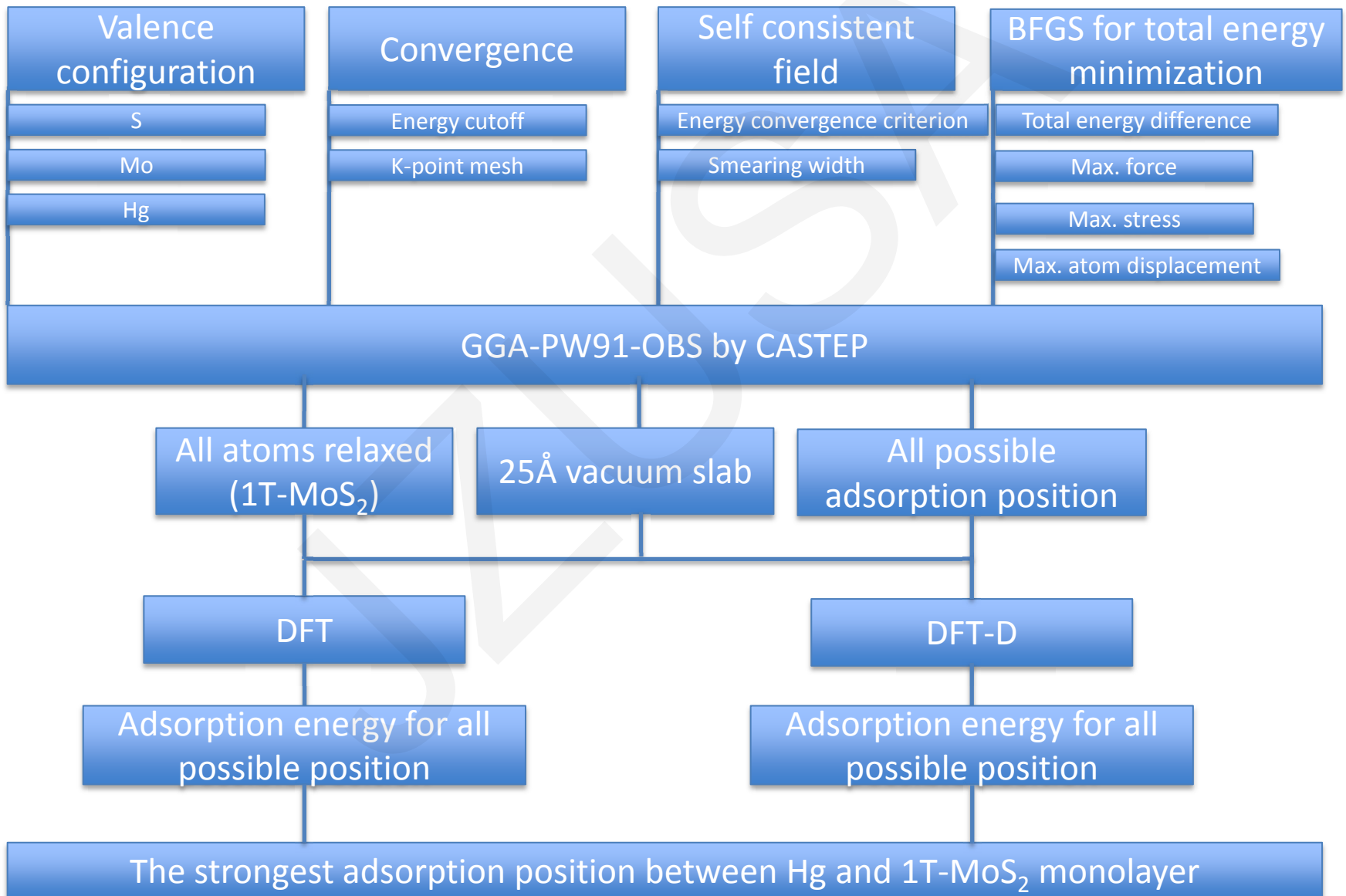
# Introduction

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<sub>2</sub> (prismatic structure of MoS<sub>2</sub>). However, the mechanism of 1T-MoS<sub>2</sub> (polytype structure of MoS<sub>2</sub>) in Hg<sup>0</sup> capture remains unexplored. In this study, density functional theory (DFT) was adopted to investigate the adsorption mechanism of Hg on a 1T-MoS<sub>2</sub> monolayer. The different possible adsorption positions on the 1T-MoS<sub>2</sub> were examined.



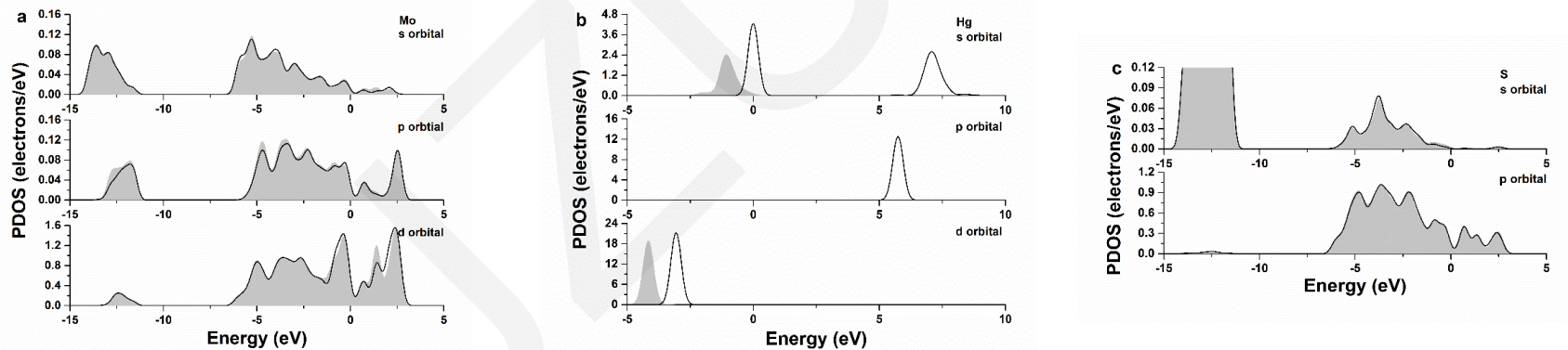
**Fig. 1.** Optimized stable structure of 1T-MoS<sub>2</sub> monolayer with adsorbed Hg atom. a. Hg atom adsorbed on the top site of a Mo atom ( $T_{Mo}$ ). b. Hg atom adsorbed on the top site of the bridge site between a S-Mo bond ( $B_{Mo-S}$ ). c. Hg atom adsorbed on the top site of a S atom in top 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  $\text{Hg}^0$  atoms and the 1T-MoS<sub>2</sub>. It was found that the  $T_{\text{Mo}}$  (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<sub>2</sub> monolayer is influenced by adjacent S and Mo atoms. The adsorbate  $\text{Hg}^0$  atom is found being oxidized on the  $T_{\text{Mo}}$  position of the 1T-MoS<sub>2</sub> 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  $\text{Hg}^0$  and the 1T-MoS<sub>2</sub> 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  $T_{\text{Mo}}$  position of 1T-MoS<sub>2</sub> 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).