

Theoretical investigation of gas molecule adsorption on WS monochalcogenide

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Detection of toxic gases (like CO, NO, H₂S, etc) has become an important issue for environment as well as human safety [1]. Carbon-based nanostructures including graphene as well as transition metal dichalcogenides (TMDs) [1] are widely studied in the literature to explore the possibility for the same. Recently, theoretical prediction on the possibility of tungsten monosulphide (WS) in the buckled configuration [2] has been reported by our group. This system shows a semi-metallic nature. Thus, in this work, we explore the possibility of CO and NO gas adsorption on WS using density functional theory (DFT) with van der Waals corrections based calculations. Adsorption energy (E_{ads}) calculations and charge transfer analysis have been performed to estimate the sensitivity towards the gas molecule. We observe that CO and NO, molecules prefer the perpendicular adsorption on 2D sheet with C and N atoms oriented towards the sheet with appreciable values of E_{ads} . Density of states study reveals that WS monolayer becomes semiconductor transition upon CO adsorption. Charge transfer theory shows that the bonding of CO and NO on WS surface occur through the 2π orbital (LUMO). Thus, the study indicates that WS monochalcogenide is sensitive towards the studied gas adsorbates and may be a potential candidate for CO and NO gas adsorption. The results await experimental validation.

References

[1]. S. Yang, C. Jiang, and S.-H. Wei, Appl. Phys. Rev. 4, 021304 (2017).

[2]. D. Pandey, A. Chakrabarti, Phys. Lett. A, 383, 2914 (2019).

Figures

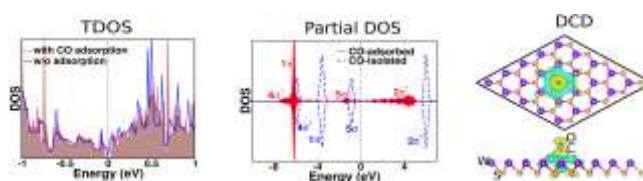


Figure 1: Density of states (DOS) and difference charge density for the CO adsorbed WS.