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Tuning the properties of Janus van der Waals hetero structures by varying interface terminations: A first principles investigation

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The ever-growing energy needs demand technological development related to photo catalysis. Conventional photo-catalytic materials suffer from low quantum efficiency, charge-recombination, and chemical back-reactions. Janus van der Waals hetero structures, are 2D materials where a metal atomic layer M is sandwiched between layers X and Y of two different chalcogen, halogen, or pnictogen atoms owing to finite out-of-plane dipole moments, and possess enhanced photocatalytic properties due to their intrinsic Rashba effect, strongly bound excitons, and strong interaction with light [1]. In this study, two dimensional (2D) GaAs/MoSSe Janus interfaces were investigated using first principles calculations. The effect of different atomic terminations on the interface stability, electronic properties and charge transfer at the interfaces were analyzed and found that conducting properties are altered with respect to different terminations. Metallic states are formed at the stable MoSSe/GaAs interface due to the presence of 2D occupied antibonding states in MoSSe and the band alignment at the interface. We demonstrate that the non-symmetric structure of MoSSe Janus material plays a key role in controlling the electronic properties of the stable Janus interface, which will be crucial deciding factor for practical applications [2]. 1. Pan, Linfeng, et al. “Boosting the performance of Cu2O photocathodes for unassisted solar water splitting devices.”Nature Catalysis 1.6 (2018): 412-420. 2. Albar, Arwa, and S. Assa Aravindh. “Emergence of metallic states at 2D MoSSe/GaAs Janus interface: a DFT study.”Journal of Physics: Condensed Matter 33.47 (2021): 475701.

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