Review of: "Two-Dimensional PtS2/MoTe2 van der Waals Heterostructure: An Efficient Potential Photocatalyst for Water Splitting"

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Potential competing interests: The author(s) declared that no potential competing interests exist.

The authors investigated the electronic band structures, and optical absorption of van der Waals heterojunction PtS2/MoTe2 by using the first-principles calculation and explored the photocatalytic hydrogen production performance.

1.The thermal stability of the heterostructure should be confirmed by molecular dynamics simulations because the photocatalytic performance does not occur at 0 K.

2.The author mentioned that the lowest binding energy is about –28.10 meV Å–2 for PM-6 stacking style. The authors should give corresponding data about these structures.

3.The author emphasized The PtS2/MoTe2 vdW heterostructure obviously can improve the optical ability of the monolayered PtS2, MoTe2 in visible regions. However this result is not sufficient to be supported by figure 6.

4.As edited that *One can see that the PtS2/MoTe2 vdW heterostructure also is a semiconductor by an indirect bandgap of 1.26 eV that the CBM is located between the Γ and M points, while the CBM exists at K point*. This sentences should be written as *while the VBM exists at K point.*

5. I'm curious about ***the PE are excited by the CB of the PtS2 and MoTe2 layers***