Exciton binding energies in group-III monochalcogenides

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The achievements in the fabrication of atomically thin layered materials [1] have enabled explorations of novel physical properties exclusively inherent to low dimensional structures. Similar to graphene, stable atomically thin layers of other materials have been prepared. Among these graphene related materials (GRMs), the transition metal dichalcogenides (TMX_2) have become pathbreaking because of their semiconducting electronic properties and distinct optical properties enabling their application in photonics and opto-electronics [2].

Apart from TMX_2, the structural related group-III monochalcogenides MX (M = Ga, In and X=S, Se, Te) have also attracted attention. These are in focus of the present study. In particular, monolayers of these materials are currently under investigation, since they have been suggested as potential photocatalysts for water splitting [3], *i.e.* a promising method for solar energy conversion by sunlight induced hydrogen reduction combined with an oxidation reaction producing H_2 and O_2. Important electronic and optical properties that determine whether the material is a suitable photocatalyst are: (i) the magnitude of the optical gap, (ii) the band off-set of the valence band maximum and the conduction band minimum with respect to the oxidation potential of $H_2O$ and the reduction potential of H^+, respectively, (iii) the exciton binding energies, and (iv) the excition lifetimes.

In the current work, we address these issues with particular emphasis on the single- and double-layers and present computational results based on density functional theory obtained using the Vienna Ab initio Simulation Package (VASP). An accurate description of the electronic and optical properties including the electron-hole interactions has been achieved by performing quasiparticle calculations within the GW approximation and solving the Bethe-Salpeter equation.

References

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Figures
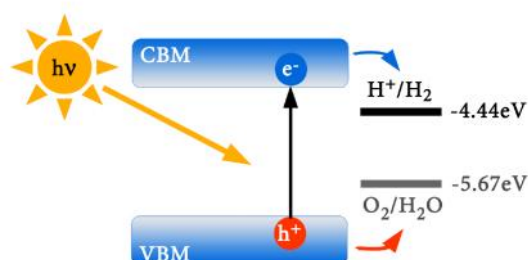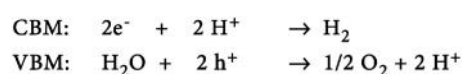
Figure 1: Schematic of the water splitting reaction using a photocatalyst. Redox potentials are given for pH=0.