Two-dimensional layered MA_2Z_4 van der Waals heterostructures for high-performance solar cells from first-principles calculations

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ABSTRACT

MA_2Z_4 two-dimensional (2D) monolayered materials (M = transition metals Mo, W; A = Si, Ge; Z = P, As, N) have gained a lot of attention in the past few years. After the first successful growth of $MoSi_2N_4$ and WSi_2N_4 in 2020 [1] by chemical vapour deposition, several monolayered materials from the same MA_2Z_4 family have been proposed and studied theoretically using density functional theory. They present several properties of interest, such as high mechanical strength [1], high piezoelectric coefficients [2], good thermal transport [2], high optoelectronic response [1, 3], and magnetism [2]. In this work we propose and study, using density functional theory, 2D layered van der Waals (vdW) heterostructures formed by MA_2Z_4 layers as candidates for the manufacturing of solar cells. By changing the atomic composition of the MA_2Z_4 layers, it is expected that the band gaps vary significantly; therefore, we propose tandem solar cells formed by heterojunctions formed by these different materials. To study their stability, we performed lattice parameter optimizations, ionic position optimizations, layer distance optimizations, molecular dynamics calculations, and calculated their vibrational modes. After confirming the stability of the proposed materials, we calculated their density of states, electronic band structure, bandgap, and optoelectronic properties, such as solar energy absorption, and carrier transport properties. This class of 2D layered vdW heterostructures shows great potential to be employed as solar cells, being competitive with other high-performance materials, such as perovskites.

References

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