

## Single-Layer Group-III Monochalcogenide Photocatalysts for Water Splitting

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The recent synthesis of single-layer GaS and GaSe opens the question of stability for other single-layer group-III monochalcogenides (MX, M = Ga and In, X = S, Se, and Te) and how the dimension reduction affects the properties of these materials. Using a first-principles design approach, we determine that the single-layer group-III monochalcogenides exhibit low formation energies and are suitable for photocatalytic water splitting. First, density-functional calculations using a van der Waals functional reveal that the monochalcogenides have formation energies similar to that of single-layer MoS<sub>2</sub>, implying the ease of mechanically extracting single-layer monochalcogenides from their layered bulk counterparts. Next, calculations using a hybrid density functional and the quasiparticle many-body  $G_0W_0$  approximation determine the conduction and valence band edge positions. Comparing the band edge positions with the redox potentials of water, shows that single-layer monochalcogenides are potential photocatalysts for water splitting. Moreover, the bandgaps, band edge positions, and the optical absorption of the single-layer monochalcogenides can be tuned by biaxial strain to increase the efficiency of solar energy conversion. Finally, our qualitative assessment of the solubility of single-layer monochalcogenides suggests their stability in solution.

- [1] H. L. Zhuang and R. G. Hennig, submitted to *Chemistry of Materials* (2013).