Photocatalysts are materials that are capable of absorbing solar energy to enable or accelerate an oxidation or reduction reaction. One such reaction is the reduction of CO₂ to hydrocarbons, which both enables the development of sustainable fuels, and facilitates managing greenhouse gas emissions. Desirable properties for a successful photocatalyst include a visible range bandgap, suitable band alignment, stability, and an appropriate binding energy to the adsorbate undergoing the reaction.

We propose a high-throughput computational approach to finding CO₂RR photocatalysts, which enables the screening of thousands of materials from the MP database within a reduced time frame. As existing adsorption workflows focus on metallic systems, we have developed a semiconductor-specific methodology to assess the adsorption capabilities of the selected materials. Combined, these two methods can significantly accelerate the discovery of novel photocatalytic systems for CO₂ reduction, an essential step in developing renewable energy technologies.

This screening procedure led to a final pool of 52 materials, 15 of which are layered. Furthermore, 43 of these materials have been previously synthesized and 9 have already been tested for CO₂ reduction.

References:

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Results

The data generated by the workflow includes adsorption energies, coordination numbers, adsorption site type, translation vectors, charge transfer and work function analysis, p-band center, orbital and elemental compositions of band edges, among others. Case study: zinc telluride

Zinc telluride is one of the 52 materials selected by the screening strategy. It has been previously used in CO₂RR photocatalytic devices. The considered adsorbates are CO and H as they are relevant species for the CO₂RR and competing hydrogen evolution reaction (HER).

Adsortion energy maps of CO (left) and H (right) on the ZnTe (1, 1, 1) 0.625 surface (top right) reveal:
- CO is strongly favored on Zn and hollow sites and strongly disfavored on Te sites
- H adsorption follows a similar trend and is generally more strongly binding than CO on this surface

Outlook

Our pre-screening filtered an initial pool of over 60,000 materials to 52 potential candidates for photocatalytic CO₂ reduction. The application of the adsorption workflow to the selected materials is expected to offer insights into the selectivity and suitability of these potential photocatalysts. This will enable us to perform more advanced studies on the most promising candidates, as well as propose them for experimental testing.