Machine Learning-Aided Band Edge Engineering in Pictogen Chalcohalides

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The rational design of photovoltaic and photocatalytic energy materials requires precise knowledge of their valence and conduction band edges positions relative to vacuum, pivotal for the efficient extraction of charge-carriers. However, exhaustive exploration of their compositional and surface-dependent effects is often computationally prohibitive.

In this work, we systematically investigate the band edge positions of pictogen chalcohalides [1,2] and their solid solutions [3] (with general formula MChX, M={Bi, Sb}, Ch={S, Se}, X={I, Br}) by combining machine learning [4,5], first-principles simulations and experimental validation.

Our results reveal that subtle compositional substitutions enable continuous tuning of the band edges by up to 0.8 eV, with a strong dependence on the exposed crystal facets. Building on these insights, we propose optimized architectures for both photovoltaic and photocatalytic applications based on MChX materials, which are further evaluated through detailed first-principles simulations and experimental validation.

References

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