UvSiB: An Open, AI-Driven Platform for Computational Screening of Photocatalysts for Solar Fuels

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Using sunlight to produce fuels and basic chemicals from abundant resources such as water, carbon dioxide, and nitrogen is one of the most promising routes towards a carbon-neutral economy. Its practical realization, however, depends on photocatalysts that simultaneously absorb visible light, separate and transport photogenerated charges efficiently, drive the desired surface reactions, and are made from inexpensive, earth-abundant elements. Finding materials that satisfy all of these requirements by experimental trial and error in an enormous chemical and structural space is slow and costly, while computational screening is usually fragmented across many tools and demands considerable expertise in simulation, machine learning, and workflow automation.

Here, we present UvSiB (Umwandlung von Sonnenenergie in Brennstoffe: Conversion of Solar Energy into Fuels), an open virtual materials-design platform for the computational identification of promising photocatalyst candidates for solar-fuel production. UvSiB integrates generative AI models, machine-learning interatomic potentials, and machine-learned property predictors into automated workflows connecting crystal-structure generation with the computational assessment of photocatalytic performance. Starting from a specified chemical system, the platform generates candidate crystal structures, evaluates their thermodynamic and dynamical stability, estimates their optical properties, constructs and selects relevant surfaces, and evaluates surface reaction energetics to assess their potential catalytic activity. Machine-learning models enable the efficient exploration and filtering of large candidate pools, reserving computationally demanding first-principles calculations for selected candidates. The results are consolidated into structured reports that connect material stability, optical properties, surface characteristics, and reaction energetics.

Each stage of the platform is implemented as a reusable building block, with computational workflows and their provenance systematically recorded to support transparency, reproducibility, restartability, and the extension of computational campaigns. A dedicated database stores curated structures and associated properties, enabling their reuse by the community. Through a user-friendly web interface, currently under development, UvSiB aims to make large-scale virtual screening more accessible to materials scientists, chemists, and physicists, including those without specialized expertise in computational materials science. Here, we present the platform's architecture, design philosophy, and current capabilities.

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