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**Band alignment at solid-liquid interfaces from GW theory combined with continuum solvation models**[1] JOHANNES LISCHNER, LARS BLUMENTHAL, MATTHIAS KAHK, PAUL TANGNEY, Imperial College London — Identifying efficient photocatalysts for the conversion of solar energy into fuels, such as hydrogen, constitutes a major challenge in the transition to a sustainable and renewable energy technology. A detailed understanding of the electronic structure of photoelectrodes, in particular the alignment of the electrode's electronic band edge positions with the relevant redox potentials of water, is required to guide experimental progress towards increased efficiencies. To address this problem, we introduce a new approach based on the combination of many-body perturbation theory within the GW approach for the electronic structure of the photoelectrode and joint density-functional theory for the description of solid-liquid interfaces. We present results for several oxide-based photoelectrodes and find good agreement with experimental band edge positions.

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