Computational Screening of Light-absorbing Materials for Photoelectrochemical Water Splitting

Efficient conversion of solar energy into electricity or fuels requires the identification of new semiconductors with optimal optical and electronic properties. We discuss the current and future role that computational screening is expected to play in this challenge. We discuss the identification of new computable descriptors characterising optimal materials performance, and we outline different search strategies in the materials screening. Finally, we describe some of the screening results obtained for perovskites, 2D materials, and for materials extracted from crystallographic databases.

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