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Computational Discovery and Design of Two-Dimensional Materials for Energy Technologies

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Our research focuses on the development of new methods and algorithms to discover materials and to describe realistic heterogeneous interfaces and the application of these methods to the discovery and design of novel two-dimensional materials for application in energy technologies and electronic devices. In this talk, I will present our data-mining approach to identify novel two-dimensional materials with low formation energies. We identify several 2D materials in the group-III monochalcogenides and the group of transition metal dichalcogenides that are suitable for photocatalytic water splitting. We show that these 2D materials in contrast to their 3D counterparts have appropriate bad gaps and alignments with the redox potentials of water, and exhibit high solvation energies, indicating their stability in aqueous environment. We show that strain can be used to tune the electronic and optical properties of these materials. Our results provide guidance for experimental synthesis efforts and future searches of materials suitable for applications in energy technologies.

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