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Aligning the band edges of Si surfaces with water redox potentials: a first-principles study[1] ERIC SCHWEGLER, Lawrence Livermore National Laboratory, TUAN ANH PHAM, Lawrence Livermore National Laboratory and Department of Chemistry UC Davis, DONGHWA LEE, Lawrence Livermore National Laboratory, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — We present first-principles calculations of the alignment between the band edges of several Si surfaces with water redox potentials using many-body perturbation theory, coupled with *ab initio* molecular dynamics simulations. Our results show that surface functionalization strongly influences the electronic properties of the interface, and indicate that a favourable alignment of band edges and water redox potentials for water splitting applications may be achieved by engineering the surface termination of the Si-based photo-electrodes. In addition, we found that in the case of hydrophilic Si surfaces, the use of simple computational schemes that neglect the detailed microscopic structure of the interfacial water layer may lead to substantial errors in predicting the alignment between the solid band edges and water redox potentials.

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