

Abstract Submitted
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Tunable Band Edges of TiO₂ via Functionalization with Phosphonic Acid Adsorbates¹ GUO LI, JESSY RIVEST, Molecular Foundry, Lawrence Berkeley National Laboratory, IAN SHARP, Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, DELIA MILLIRON, Molecular Foundry, Lawrence Berkeley National Laboratory, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory; Department of Physics, UC-Berkeley — The deliberate design of semiconductor surfaces with band edge energies optimal for electro- or photoelectrochemical applications is a grand challenge. We examine the extent that the band edges of anatase TiO₂(101) can be effectively tuned via molecular adsorption on its surface. Using density functional theory, we compute TiO₂ band edge energies for a series of phosphonic acid molecules, whose intrinsic dipole moments are significantly different in both magnitude and direction. The results reveal that the molecule-substrate binding leads to a large induced dipole moment, and the induced dipole upon adsorption varies with the binding nature and configuration. Repulsive dipole-dipole interactions between molecules lead to a striking coverage-dependence of the effective dipole moments. Interestingly, computed band edge shifts in TiO₂ are in excellent agreement with the experimentally measured work-function changes. Implications for the role of such adsorbates on photoelectrochemical devices will be discussed.

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