Abstract Submitted
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First Principles Study of the Electronic Structure of Organic Adsorbates on Cleaved GaP Surfaces[1] MIN YU, PETER DOAK, JEFFREY NEATON, Lawrence Berkeley National Laboratory — We report a first principles calculations of structural, electronic, and spectroscopic properties of organic molecules, such as ethylene and benzene, adsorbed on cleaved GaP (110) surface to assess their potential to allow controlled coupling and to modify charge transport between light absorbing semiconductors and catalysts for applications in artificial photosynthesis. We compute adsorbate geometries, binding energetics, surface band structures, constant current scanning tunneling microscopy images, and electronic energy level alignment of organic molecules on GaP surfaces using density functional theory and many-body perturbation theory within the GW approximation. We quantify the impact of coverage, interface dipoles, hybridization, and nonlocal polarization effects on level alignment, and validate our understanding through direct comparison recent measurements. Work supported by JCAP and computational resources provided by NERSC.

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