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First-Principles Studies of Structure and Energy Level Alignment of Thiophene Assemblies on Methyl-Terminated Si(111) MIN YU, PETER DOAK, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Adsorption of organic molecules on semiconductor photocatalysts has attracted significant attention for energy conversion applications. In this work, we use density functional theory and many-body perturbation theory within the GW approximation to study the geometry, binding energetics, and energy level alignment of a model ligand, thiophene (C4H4S), chemisorbed via a C-Si bond on methyl-terminated silicon(111) substrates. We quantify the impact of coverage, interface dipoles, hybridization, and polarization effects on level alignment. For sufficiently weakly-coupled frontier orbitals, we explore the extent to which the self-energy change upon adsorption relative to the gas phase is dominated by nonlocal electrostatic polarization effects [1]. The implications of our results for other thiophene-related ligands, and future spectroscopic experiments, will be thoroughly discussed. We acknowledge DOE for support through JCAP, and NERSC for computational resources.

[1] J. B. Neaton, M. S. Hybertsen and S. G. Louie, Phys. Rev. Lett. 97, 216405 (2006).

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