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Understanding electronic properties at organic/silicon interfaces from first principles

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Organic/inorganic interfaces often possess properties that are significantly different from those of the organic molecules and the inorganic substrate that comprise them, due to both inter- molecular and molecule-substrate interactions. In this talk, I show how we explore such electronic effects using first principles calculations of prototypical silicon/organic interfaces. I focus on dipole depolarization effects, demonstrated for benzene derivatives on Si(111), and on interface-induced gap states, demonstrated on alkyl chains on Si (111). By comparing the results to both experiment and phenomenological models, we rationalize these effects and predict their manifestation in a range of organic electronic structures and devices.