

Photoabsorption of adsorbed azobenzene monolayers: impact of graphene substrate

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We use density-functional theory and many-body perturbation theory to study the impact of the graphene substrate on the photo-absorption properties of *trans*- and *cis*-azobenzene monolayers. The molecules are weakly bound to graphene, and their orbitals are essentially not hybridized with bands of the substrate. Yet graphene remarkably modulates the absorption spectra of the adsorbates. Firstly, it influences excitation energies via (i) substrate polarization reducing the band-gap of azobenzene and (ii) enhanced dielectric screening, which weakens the attractive interaction between electrons and holes. Secondly, graphene activates intermolecular excitations, which are dark in the isolated monolayers. Our results demonstrate that the photoisomerization process of weakly adsorbed azobenzene undergoes notable changes on the carbon-based substrate compared to the isolated monolayers.