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The Effect of van der Waals Interactions on the Sexithiophene Adsorption on Ag(110)[1] JERONIMO MATOS, TOMAS ROJAS, ABDELKADER KARA, Department of Physics, University of Central Florida — We use density functional theory to study the adsorption of Sexithiophene (6T) on Ag(110). Special attention is given for exploring the effects of van der Waals interactions on the adsorption geometry and energy using vdW-DF family functionals. The 6T molecule is found to bind to the Ag(110) surface via two orientations, with the long molecular axis parallel to the [001] and [110] directions. Including van der Waals interactions resulted in a substantial increase in the binding energy (from 0.6 eV to 4 eV), while the binding height is slightly modified (from 3.1 Å to 2.75 Å). Both the binding energies and heights show significant variations depending on the vdW functional used: the opt-type functionals (optB86, optB88, optPBE) further enhance the adsorption energy when compared to those obtained using PBE, revPBE, or rPW86 functionals. Upon adsorption, there is a small, however, noticeable broadening and a shift (towards higher binding energy) in the position of the d-band center of the substrate surface atoms is observed. Note that, the absence of charge transfer, interfacial states, changes in the atomic structure of the molecule or the substrate suggests that the bonding characteristic of the 6T/Ag(110) system can be categorized as weak chemisorption or strong physisorption.

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