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Adsorption and diffusion of sexithiophene on Ag(110) JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — We use density functional theory (DFT-PBE-PAW) to calculate the absorption of sexithiophene (6T) molecules on Ag (110). Our results show that these molecules absorb 3 Å above the surface with a binding energy of about 0.64 eV/molecule. The internal structure of the molecule as well as the substrate atomic positions was not altered by the absorption. The energy barrier for diffusion of a 6T molecule along the channel was found to be 66 meV. Analysis of the densities of state shows little modification of the electronic structure of the substrate. Without inclusion of Van der Waals interactions, our results point to a weak chemisorption or a strong physisorption of 6T on Ag (110).

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