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Effects of Peptide Adsorption on the Electronic Properties of Graphene BRAHIM AKDIM, ZHIFENG KUANG, SANG KIM, RAJESH NAIK, BARRY FARMER, AFRL, TIFFANY WALSH, University of Warwick, RUTH PACHTER, AFRL — In this work we aim to explain the increase in the electrical conductance in a single-layer graphene (SLG) field-effect transistor (FET) upon binding the peptide HSSYWYAFNNKT, which we previously demonstrated. The adsorption of the peptide onto the SLG has been carefully modeled by applying empirical molecular dynamics simulations with the AMOEBA force-field. The peptide adsorbed SLG structure demonstrates $\pi - \pi$ stacking with aromatic amino acids, namely His,Tyr, Thr and Ph. Based on this large-scale peptide-SLG system, calculations on the electron transport using the nonequilibrium Green's function formalism at the extended Huckel level were carried out. Transmission eigenchannels and spectra, projected density of states, effects of modeling realistic leads (gold vs. graphene) and $I - V$ characteristics will be discussed in detail. In this context, suppositions as to the mechanism of increased conductance for the peptide-SLG FET will be proposed.

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