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Surface-enhanced Raman spectroscopic studies of the Au-pentacene interface: a combined experimental and theoretical investigation[1] SUCHISMITA GUHA, DANISH ADIL, University of Missouri, Columbia — A large enhancement in the Raman intensity due to surface-enhanced Raman scattering (SERS) is observed from pentacene when probed through the Au contact in organic field-effect transistor (OFET) structures. The SERS spectrum is shown to exhibit a high sensitivity to disorder introduced in the pentacene film by Au atoms. The Raman signature of the metal-semiconductor interface in pentacene OFETs is calculated within density-functional theory by explicitly considering the Au-pentacene interaction. The observed enhancement in the 1380 cm^{-1} and the 1560 cm^{-1} regions of the experimental Raman spectrum of pentacene is successfully modeled by Au-pentacene complexes, giving insights into the nature of disorder in the pentacene sp^2 network. Raman maps across the pentacene-Au interface provide a powerful visualization tool for correlating the device performance, namely changes in the threshold voltages upon bias stress, to structural changes of the molecule. Unlike high-operating voltage OFETs, low-operating voltage OFETs show no change in the SERS spectra before and after the application of a bias stress, concurrent with no degradation in their threshold voltage.

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