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Ab initio calculation of transmission and I-V curve for π-stacked polythiophene layers sandwiched between gold electrodes. SERGEY FALEEV, FRANCOIS LEONARD, Sandia National Laboratories, MARK VAN SCHILFGAARDE, Arizona State University — We have applied an implementation of recently developed [Faleev et. al. PRB 71, 195422 (2005)] non-equilibrium Green's Function method in framework of the tight-binding LMTO approach in its atomic sphere approximation to calculate the transmission function and I-V curves of π-stacked polythiophene layers sandwiched between Au(111) electrodes. Our approach is a fully *ab initio* all-electron approach that treats the central region and electrodes on equal footing. To the best of our knowledge, this is first application of an *ab initio* approach to calculation of transport properties of multiple polymer layers arranged *parallel* to the metal surface, as opposed to previously studied systems of a small molecule or oligomer attached at both ends to the electrodes. We found that for a number of layers L $>$ 1, an increasingly pronounced dip in the transmission function is formed at energies from E_F to E_F + 0.5 eV, reflecting the semiconductor nature of a polythiophene multilayer film. The zero-bias conductance of the film exhibits large-L asymptotic behavior $\sigma \approx G_0 \exp(-1.2(L-5))$, starting with L $\approx$ 6 that can be seen as a thickness of the thin polythiophene film at which a metal-semiconductor transition occurs. For L = 1, the current depends linearly on applied voltage, while at L $>$ 1, current is non-linear, reflecting strong bias and energy dependence of the transmission function.

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