

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Ab initio calculation of transmission and I-V curve for  $\pi$ -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  $\pi$ -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.

Sergey Faleev  
Sandia National Laboratories

Date submitted: 03 Dec 2006

Electronic form version 1.4