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The injection barrier at a metal/organic interface D. H. DUNLAP, TIANJIAN LU, University of New Mexico — The landscape for the thermionic injection of electrons from a metal into a molecularly doped polymer is energetically disordered as a result of inhomogeneous electric fields coming from the non-uniform charging of dopant molecules in the vicinity of the metal/organic interface. This comprises an electric dipole (double - ) layer. We have determined the equilibrium composition of the dipole layer by simulated annealing, in order to study its influence on injection. We find that an electron must surmount an energetic barrier in order to escape into the organic, even when the LUMO level of the dopants is aligned with the Fermi level of the metal. For typical dopant densities, this barrier is on the order of 0.5 eV.

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