Transport through Self-Assembled Monolayer Molecular Junctions: Role of In-Plane Dephasing

JONATAN DUBI, Ben-Gurion University of the Negev — Self-assembled-monolayer (SAM) molecular junctions (MJs) constitute a promising building block candidate for future molecular electronic devices. Transport properties of SAM-MJs are usually calculated using either the phenomenological Simmons model, or a fully-coherent transport theory, employing the SAMs periodicity. As I will show, the standard theory seems to have some discrepancy with experimental observations. To overcome these discrepancies, I suggest that dephasing plays an important role in determining the transport properties of SAM-MJs. I will present an approach for calculating the transport properties of SAM-MJs that inherently takes into account in-plane dephasing in the electron motion as it traverses the SAM plane. The approach describes well the two hallmarks of transport through SAM-MJs, namely the exponential decay of current with molecular chain length and the reduction of the current per molecule as compared to single-molecule junctions. Specifically, I will show that dephasing leads to an exponential decay of the current as a function of molecular length, even for resonant tunneling, where the fully coherent calculation shows little or no length-dependence of the current. The dephasing is also shown to lead to a substantial reduction of the current in a