

Abstract Submitted
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Theory of tunneling and electron transport through single molecules of polyaniline¹ OTTO SANKEY, MYEONG LEE, GIL SPEYER, Arizona State University — Polyaniline is a linear organic polymer used often in battery devices, films, and organic electrodes, and it exhibits a dramatic increase in conductivity due to electrochemical oxidation or acidic treatment. The polymer chain has different bonding configurations depending on the oxidation state — they include leucoemeraldine, emeraldine, and pernigraniline bases and their salts. Most forms are semiconducting and electron transport through these forms as single molecules is expected to occur via a tunneling mechanism. We have computed the complex bandstructure (which include imaginary k-vectors to allow for tunneling) of the semiconducting forms to gain insight into the expected length dependence of the electron tunneling current ($\sim e^{-\beta L}$) and the energy dependence of the decay parameter β . Model calculations of the I-V curves for metal/single-molecule/metal molecular electronics geometries will be discussed (the metal is gold). The electron transport calculations use DFT Green's function scattering methods.

¹This work in collaboration with the ASU NSF/NIRT team

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