

Abstract Submitted  
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**Calculations of Electron Transport through Radicals** MANUEL

SMEU, McGill University, GINO DILABIO, National Institute for Nanotechnology — Organic radicals are of interest in molecular electronics because a singly occupied molecular orbital (SOMO) would have a higher energy than its doubly occupied analog, suggesting they might make better conductors. The unpaired electron present in a radical leads to degeneracy splitting in other energy levels and such molecules may act as spin filters. Our study employs first principles transport calculations that are performed using a combination of density functional theory and a non-equilibrium Green's function technique. The conductance of 1,4-benzenediamine (BDA) molecules bridging two Au electrodes was modeled. These molecules were substituted in the 2-position with: -CH<sub>3</sub>, -NH<sub>2</sub>, and -OH; as well as with their radical analogs: -CH<sub>2</sub>, -NH, and -O, all of which have  $\pi$ -type SOMOs. The conductance of a radical with a  $\sigma$ -type SOMO was also calculated from a BDA molecule with the H atom in the 2-position removed. Comparing the transmission spectra for these species will yield insight into the nature of electron transport through radicals vs. transport through their reduced form as well as the nature of transport through  $\pi$ - and  $\sigma$ -type molecular orbitals.

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