Effects of dephasing on molecular conduction\textsuperscript{1} JESSE MAASSEN, FERDOWS ZAHID, HONG GUO, Centre for the Physics of Materials and Department of Physics, McGill University, Montreal, Canada — In this work, we theoretically investigate effects of dephasing on electron transport in molecular wires. The quantum transport analysis is carried out using the density functional theory (DFT) combined with the non-equilibrium Green’s function framework (NEGF). The dephasing effect is included at a phenomenological level by introducing fictitious voltage probes to the NEGF-DFT formalism that mimics the randomisation of quantum phase information of the charge carriers. For three systems: (i) a 1,4-benzenedithiol (BDT) molecule connected to Al(001) leads; (ii) an atomic gold chain in contact with Au(001) leads; and (iii) a very narrow Al(001) nanowire, our results indicate that there are two behaviours. When the wires are not conductive as (i,ii), the dephasing effects can increase conduction for a range of system parameters; while for conducting systems (iii), the effect is opposite. These effects can be understood from a quantum interference point of view. We also compare results for two different models on how the phenomenological dephasing effects are introduced into the NEGF-DFT formalism.

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