Hartree Fock calculation of molecular wires via Non-equilibrium Green's function approach

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Electron transport through molecular wires sandwiched by semi-infinite electrodes has attracted much interest amongst theorists.As a first step towards using electronic structure methodology in conductance calculations, we study the NEGF Hartree-Fock (HF) theory of conductance of molecular wires. By doing the calculations with both DFT and HF methods, we aim to assess the importance of self-interaction in the treatment of conductance.