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Electron Propagator Calculations on Molecular Wires[1] YURI DAHNOVSKY, Department of Physics & Astronomy, University of Wyoming, VYACHESLAV ZAKRZHEWSKI, Department of Chemistry, Kansas State University, ALEXEI KLETSOV, Department of Physics & Astronomy, University of Wyoming, VINCE ORTIZ, Department of Chemistry, Kansas State University, YURI DAHNOVSKY AND ALEXEI KLETSOV TEAM, VINCE ORTIZ AND VYACHESLAV ZAKRZHEWSKI TEAM — Several molecular wires are studied by an *electron propagator* method. This *ab initio* method does not include any adjustable parameter or an additional potential introduced into a Hamiltonian. Such an approach is based on an accurate calculation of infinite series of diagrams rigorously describing the electron correlation in a bridge molecule. In this work we compute nonequilibrium Keldysh functions in order to find the dependence of current on applied voltage for particular molecular wires. Quantum chemical calculations are performed for several molecular bridges. The extended molecule approach is adopted. Results are compared with available experimental data and other quantum chemical approaches, in particular those based on density functional theory.

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