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Active Transport Orbitals in Electron Propagator Calculations on Molecular Wires. YURI DAHNOVSKY, Department of Physcs & Astronomy, University of Wyoming, V.G. ZAKRZEWSKI, Department of Chemistry, Kansas State University, ALEXEY KLETSOV, Department of Electrical Engineering, University of Wyoming, J.V. ORTIZ, Department of Chemistry, Kansas State University, YURI DAHNOVSKY AND ALEXEY KLETSOV COLLABORATION, V. J. ORTIZ AND V. G. ZAKRZEWSKI COLLABORATION — *Ab initio* electron propagator methodology may be applied to the calculation of electrical current through a molecular wire. A new theoretical approach is developed for the calculation of the retarded and advanced Green functions in terms of the electron propagator matrix for the bridge molecule. The calculation of the current requires integration in a complex half-plane for a trace that involves terminal and Green function matrices. Because the Green function matrices have complex poles represented by matrices, a special scheme is developed to express these "matrix poles" in terms of ordinary poles. An expression for the current is derived for a terminal matrix of arbitrary rank. For multi-terminal terminals, the analytical expression for the current is given in terms of pole strengths, poles and terminal matrix elements of the electron propagator. It is shown that Dyson orbitals with high pole strengths and overlaps with terminal orbitals are most responsible for conduction of electrical current.

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