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Complex band structure of a metallic nanowire under plane-wave nonlocal pseudopotential Hamiltonian and non equilibrium quantum transport calculations MAIA G. VERGNIORY, LIN-WANG WANG, Lawrence Berkeley National Laboratory — We present ab initio calculations of the complex band structure of a copper and gold nanowire with a nonlocal plane-wave pseudopotential Hamiltonians. This new method allows us to calculate the evanescent states exactly using plane waves of any metallic electrode. The calculation of the evanescent states is important for quantum transport calculations when the transmisson energy is close to a band structure minimun. Nonlocal pseudopotential effects are introduced using the Kleinman-Bylander implementation. Using the method in Ref[1], where the quantum transport is calculated by means of the exact scattering states using plane waves basis set, we have calculated the nonequilibrium transmission coefficient and conductivities of a di-thiol-benzene (DBT) and other molecules connected by two Cu or Au nano wires.

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