ELECTRONIC CONDUCTANCE VIA SODIUM CHAINS: A WAVE FUNCTION MATCHING THEORY

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A model calculation is presented for the quantum transport of electrons between leads of a given element via intermediate nanojunctions made up of finite one-dimensional atomic chains of another element. The electronic conductance is calculated using the wave function matching theory, to derive the transmission and reflection scattering matrices familiar in the Landauer-Büttiker formalism. In particular, we apply our model to calculate numerically the electronic transport in mono-atomic linear sodium chains (MALSC) as nanojunctions between cesium leads. The electronic dynamics for the system are calculated using the Slater-Koster tight-binding approximation, with appropriate tight-binding parameters. Our theoretical approach is quite general for varying MALSC lengths and as a result correctly reproduces the even-odd conductance oscillation behavior. It provides, further, an efficient tool for both electronic transport calculations for a wide range of nanomaterial chain systems.

9.7 cm

13.4 cm

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