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Electron transport described in terms of the Dirac equation MATTHIAS ERNZERHOF, FRANCOIS GOYER, Department of Chemistry, University of Montreal — Starting from the Hückel Hamiltonian of finite, unsaturated hydrocarbon chains (ethylene, allyl radical, butadiene, pentadienyl radical, hexatriene, etc.), we perform a simple unitary transformation and obtain a Dirac matrix Hamiltonian. Thus already these small systems are described exactly in terms of the Dirac equation, the continuum limit of which yields the one-dimensional Dirac Hamiltonian. Using the source-sink potential method [1,2], complex potentials are introduced into the Dirac Hamiltonian to model infinite metal contacts. The electron-transport properties are then calculated and interpreted in terms of the Dirac Hamiltonian. Furthermore, we illustrate how the findings for short carbon chains carry over to a certain class of square graphene sheets.
[1] F. Goyer, M. Ernzerhof, M. Zhuang, J. Chem. Phys. 126, 144104 (2007).
[2] M. Ernzerhof, J. Chem. Phys. 127, 204709 (2007).

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