

Structural and electronic properties of molybdenum chalcogenide nanowires

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We combine *ab initio* density functional and quantum transport calculations based on the nonequilibrium Green's function formalism to compare structural, electronic, and transport properties of $\text{Mo}_6\text{S}_{6-x}\text{I}_x$ nanowires with carbon nanotubes. We find systems with $x=2$ to be particularly stable and rigid, with their electronic structure and conductance close to that of metallic (13,13) single-wall carbon nanotubes. $\text{Mo}_6\text{S}_{6-x}\text{I}_x$ nanowires are conductive irrespective of their structure, more easily separable than carbon nanotubes, and capable of forming ideal contact to Au leads through thio groups.

Figure 1: (a) Structure of $\text{Mo}_6\text{S}_4\text{I}_2$ nanowires arranged on a simple hexagonal lattice in a plane normal to the wire axes. (b) Contour plot of the nanowire binding energy in this lattice as a function of the wire orientation and separation.

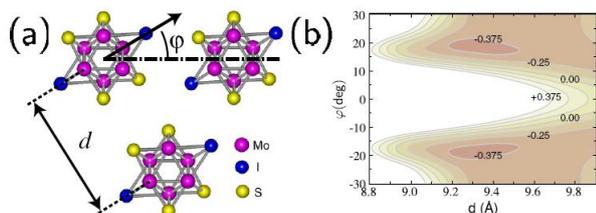


Figure 2: Electronic properties of a $\text{Mo}_6\text{S}_{6-x}\text{I}_x$ nanowires in comparison to a (13,13) carbon nanotube. Left column: band structure, middle column: density of states, right column: quantum conductance. $E=0$ corresponds to Fermi level.

