

# Structural and electronic properties of molybdenum chalcogenide nanowires

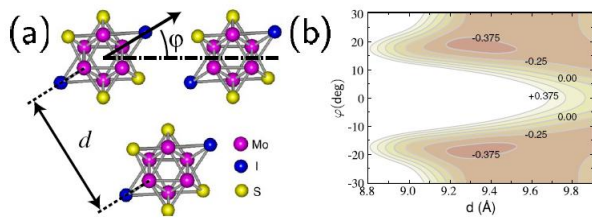
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We combine *ab initio* density functional and quantum transport calculations based on the nonequilibrium Green's function formalism to compare structural, electronic, and transport properties of  $\text{Mo}_6\text{S}_{6-x}\text{I}_x$  nanowires with 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.

