Replicating carbon nanotubes with molybdenum chalcogenide nanowires

TENG YANG, DAVID TOMANEK, Michigan State University, IGOR POPOV, GOTTHARD SEIFERT, TU Dresden — In an attempt to design chemically stable and easily separable one-dimensional conductors, we performed \textit{ab initio} Density Functional calculations for Mo$_6$S$_{6-x}$I$_x$ nanowires with a varying concentration of iodine. Such Chevrel like systems have been synthesized before, but had necessitated alkali counter-ions for stabilization. The backbone of our nanowires consists of Mo$_6$ octahedra structures, covered by I and S atoms. We find the stoichiometry with $x = 2$ to be preferred on energy grounds. Our results suggest these nanowires to be not only structurally rigid, but also to be rather easily separable. The electronic structure of these nanowires strongly resembles that of semi-metallic carbon nanotubes, with two crossing bands giving rise to a constant density of states, flanked by a pair of van Hove singularities near the Fermi level. Since the semi-metallic nature of these nanowires is robust, these systems may offer a viable alternative to carbon nanotubes, where conductivity strongly depends on chirality.

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