

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Replicating carbon nanotubes with molybdenum chalcogenide nanowires¹ 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 *ab initio* Density Functional calculations for $\text{Mo}_6\text{S}_{6-x}\text{I}_x$ 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.

¹Supported by NSF NSEC grant EEC-425826 and NSF NIRT grant ECS-0506309.

Teng Yang
Michigan State University

Date submitted: 29 Nov 2006

Electronic form version 1.4