

Abstract Submitted
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Structural and Electronic Properties of $\text{Mo}_6\text{S}_x\text{I}_{9-x}$ Nanowires.¹

TENG YANG, Michigan State University, JIPING LI, Michigan State University, SAVAS BERBER, University of Tsukuba, DAVID TOMANEK, Michigan State University — We investigate the equilibrium geometry and electronic structure of recently synthesized $\text{Mo}_6\text{S}_x\text{I}_{9-x}$ nanowires using *ab initio* Density Functional calculations. Our structure optimization calculations suggest a well-defined atomic structure within these nanowires, which are energetically unusually stable in view of their sub-nanometer diameter. For particular stoichiometries, we find the $\text{Mo}_6\text{S}_x\text{I}_{9-x}$ nanowires to be rather soft with respect to axial compression, and also to be metallic. We characterize the quantum conductance in these nanowires using a self-consistent nonequilibrium Green's function approach within the Landauer-Buttiker formalism. We find the charge density near the Fermi level to be delocalized along the wires, suggesting a high polarizability. For particular metastable geometries, the nanowires also exhibit a magnetic instability. Combination of atomic-scale perfection with a high structural stability and unusual electronic and transport properties lends itself to potential applications of these nanowires as unique building blocks in hierarchically assembled electronic nanocircuits.

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