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Structural ordering, electronic and magnetic properties of bundled $Mo_6S_{9-x}I_x$ nanowires[1] SEOUNG-HUN KANG, YOUNG-KYUN KWON, Kyung Hee University, DAVID TOMÁNEK, Michigan State University — We use *ab initio* density functional theory calculations to determine the effect of bundling on the equilibrium structure, electronic and magnetic properties of $Mo_6S_{9-x}I_x$ nanowires with $x = 0, 3, 4.5, 6$. Each unit cell of these systems contains two S- and I-decorated Mo_6 clusters that are connected by S_3 linkages to form an ordered linear array. Due to the bi-stability of the sulfur linkages, the total energy of the nanowires exhibits typically many minima as a function of the wire length. We find the optimum inter-wire distance to depend sensitively on the orientation of the wires, but only weakly on x. Structural order is expected in bundles with $x = 0$ and $x = 6$, since there is no disorder in the decoration of the Mo clusters. In bundles with other stoichiometries we expect structural disorder to occur. We find that the nanowires can be switched from metallic to semiconducting behavior by applying axial stress. Selected stable and many more unstable atomic arrangements cause ferromagnetic behavior in nanowire bundles.

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