N-004

Structural ordering, electronic and magnetic properties of bundled $Mo_6S_{9-x}I_x$ nanowires

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We use *ab initio* density functional theory 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 $Mo_6S_{6-x}I_x$ clusters 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 that nanowires can switch over from metallic to semiconducting by applying axial stress. 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 the optimum inter-wire distance to depend sensitively on the orientation of the wires, but only weakly on x. It is also found that the electronic properties of nanowires are affected strongly due to bundling of nanowires exhibiting very unusual Fermi surfaces. Furthermore, ferromagnetic behaviors are observed in selected stable and many more unstable atomic arrangements in nanowire bundles.