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Compositional and magnetic ordering in $\text{Mo}_6\text{S}_{9-x}\text{I}_x$ nanowires¹

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— We investigate the effect of atomic ordering and geometry on the relative stability and electronic as well as magnetic structure of $\text{Mo}_6\text{S}_{9-x}\text{I}_x$ nanowires using *ab initio* Spin Density Functional calculations. The skeleton of these unusually stable nanowires consists of Mo octahedra, which are decorated with S and I atoms and connected by sulfur bridges. These sulfur bridges turn out to be bi-stable, providing the nanowires with the unusual capability to stretch by 20% at no energy cost. Depending on the degree the nanowires have been stretched, they may reversibly acquire or lose their magnetic moment. The ordering of the decorating atoms, observed in these nanowires, reflects our finding that the total energy depends sensitively on the atomic arrangement at a given stoichiometry.

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