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Interplay between structural and electronic properties of bundled $Mo_6S_{9-x}I_x$ nanowires: an *ab initio* study SEOUNG-HUN KANG, YOUNG-KYUN KWON, Kyung Hee University, DAVID TOMANEK, Michigan State University — We use first principles density functional theory to investigate the structural, electronic and magnetic properties of isolated and bundled $Mo_6S_{9-x}I_x$ nanowires with $x = 3, 4.5$, and 6. The skeleton of these nanowires consists of linear arrays of Mo_6 octahedra decorated with S and I atoms that are connected by flexible S_3 linkages. Due to the bi-stability of each sulfur linkage, free-standing and bundled nanowires are capable of stretching or compressing axially at almost no energy cost, giving rise to many structural minima. We explore the structural stability, elastic behavior and electronic structure at all these minima for different compositions. We find that axial strain and inter-wire interaction in bundles modify significantly the electronic structure. Most intriguing changes occur in nanowires with $x = 4.5$ and 6, which change from metal to semiconductor or undergo a magnetic transition upon axially stretching or compressing the nanowires or upon changing the inter-wire separation.

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