**The structural and electronic properties of Mo6S3I6 nanowires by theoretical compositional arrangement**

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The structural, electronic, magnetic properties of molybdenum-based nanowires have been actively investigated for their potential applications as nanodevices; but further developments are retarded due to the lack of knowledge on the exact electronic and atomic structures of Mo6S3I6. For further development of Mo6S3I6 nanowire devices, we propose possible atomic structures and the corresponding electronic properties of Mo6S3I6 nanowires based on our density functional theory calculations. We scanned various combinations of atomic structures by changing the decorative positions of sulfur and iodine linked to two Mo6 octahedral. As a result, we found two stable local energy minimum structures characterized by elongation of S3 linkage; and propose, based on the two stable structures, possible structures of twenty-eight atomic models according to the sulfur saturation in bridging plane. We calculated band structures of the newly proposed atomic models and finally found three atomic models of conductors. According to our compositional ordering structural analysis, we concluded (i) periodic distortion of the bond lengths influences the behavior of the electrons in a system, (ii) role of sulfur atoms in bridging plane is important for intramolecular charge transport by the delocalized charge differences, and (iii) electronic band gap energy is proportional to the integrated Mo-S bonding orbital energy.

