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Strong orientation dependence of electronic properties of Antimony Selenide (Sb_2Se_3) nanostructures RAJASEKARAKUMAR VADAPOO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA, SRIDEVI KRISHNAN, Institute of Materials Science, University of Connecticut, CT 06269, USA, HULUSI YILMAZ, Dept. Of Engineering, Zaman University, Phnom Penh, Cambodia, CARLOS MARIN, Institute for Functional Nanomaterials and Department of General Engineering, University of Puerto Rico, Mayaguez, PR 00681, USA — Antimony Selenide has applications in thermoelectric, photovoltaic and optical storage. Recently, it was demonstrated that bulk material under high pressure becomes a topological insulator and further undergoes insulator to metal to superconducting transitions. The Sb_2Se_3 nanostructures reported so far exhibit direct bandgaps, whereas the bulk has an indirect gap. Considering different crystallographic orientations of synthesized nanostructures and the anisotropic nature of its structure, we have studied the influence of orientation on their electronic behavior. Using first principle methods, we explore the stability of nanowires in different orientations and its influence on electronic structure. We find confinement effects for the narrower nanostructures, whereas the [001] orientation showed a reduced bandgap. This anomalous behavior is discussed considering that bandgap reduction could be attributed to recent experimental findings of a insulator-metal transition, which is related to topological quantum transition. The surface reconstructions show similarities to the distortion of polyhedras occurring in bulk Sb_2Se_3 under high pressure, which are related to the insulator-metal transition and superconductivity at 8.0 K.

> Rajasekarakumar Vadapoo Geophysical Laboratory, Washington, DC 20015, USA.

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