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Strain-induced semi-metal to semiconductor transition and strong enhancement in thermopower of TiS_2[1] ATANU SAMANTA, TRIBHUWAN PANDEY, ABHISHEK K. SINGH, Materials Research Centre, Indian Institute of Science, Bangalore-560012 — Electronic properties of transition-metal dichalcogenides (TMDs) (MX_2, where M = Mo, W and X = S, Se, Te) are very sensitive to the applied pressure/strain, causing a semiconductor to metal transition. Using first principles density functional theory calculations, we demonstrate that bulk TiS_2 changes from semi-metal to semi-conducting electronic phase upon application of uniform biaxial strain. This phase transition is responsible for the charge transfer from Ti to S and reduces the overlap between Ti-(d) and S-(p) orbitals. The transport calculations show a three-fold enhancement in thermopower for both p- and n-type TiS_2 due to opening of band gap along with changes in dispersion of bands. The electrical conductivity and thermopower shows a large anisotropy due to the difference in the effective masses along the in-plane and out-of-plane directions. We further demonstrate that the enhancement of thermoelectric performance, can also be achieved by doping TiS_2 with larger iso-electronic elements such as Zr or Hf at the Ti sites.

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Atanu Samanta
Materials Research Centre, Indian Institute of Science, Bangalore-560012

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