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The Layered Transition Metal Dichalcogenides as Materials for Storage Clean Energy: Ab initio Investigations

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Abstract : Transition metal dichalcogenides have potential applications in power generation devices that convert waste heat into electric current by the so-called Seebeck and Hall effects thus providing an alternative energy technology to reduce the dependence on traditional fossil fuels. In this study, the thermoelectric properties of 1T and 2HTaX2 (X= S or Se) dichalcogenide superconductors have been computed using the semi-classical Boltzmann theory. Technologically, the task is to fabricate suitable materials with high efficiency. It is found that 2HTaS2 possesses the largest value of figure of merit ZT= 1.27 at 175 K. From a scientific point of view, we aim to model the underlying materials properties and in particular the transport phenomena as mediated by electrons and lattice vibrations responsible for superconductivity, Charge Density Waves (CDW) and metal/insulator transitions as function of temperature. The goal of the present work is to develop an understanding of the superconductivity of these selected materials using the transport properties at the fundamental level.

Keywords : Ab initio, High efficiency, Power generation devices, Transition metal dichalcogenides
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