

Abstract Submitted
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Electronic structure and thermoelectric properties of $(\text{PbSe})_m/(\text{SnSe})_n$ superlattice: A first principles study¹ DUC CUONG DO, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 680-749, South Korea, S.H. RHIM, SOON CHEOL HONG, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Ulsan 680-749, South Korea — Figure of merit (ZT) of thermoelectric materials can be enhanced by lowering thermal conductivity or/and increasing electrical conductivity. The extremely high ZT of layered structure SnSe ² opened up a new direction in study of thermoelectricity due to its low thermal conductivity, which, however, is limited to high temperature. Here, we performed first principles density functional calculations to explore room-temperature thermoelectricity. We consider $(\text{PbSe})_m/(\text{SnSe})_n$ superlattices with different period, whose quantum well structure is expected to increase electrical conductivity by modulation of charge doping at interface. Calculations of Seebeck coefficients for the superlattices are presented.

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