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High pressure effect on structure, electronic structure and thermoelectric properties of MoS_2[1] HUAIHONG GUO, TENG YANG, ZHIDONG ZHANG, Institute of Metal Research, Chinese academy of Sciences — We systematically study high pressure effect on the shape of the unit cell, electronic structure and transport properties of 2H-MoS_2, based on density functional calculations and the Boltzmann transport theory. Under pressure, the cross-plane lattice size decreases much faster than the in-plane one, due to the van der Waals interaction, and the size reduction becomes more difficult as external pressure exceeds 20 GPa, agreeing with experimental observation. A conversion from van der Waals to covalent bonding is seen in the calculated charge density and obtial projection of the wave functions. Concurrently, the dependence of band structure on pressure shows that a transition from semiconductor to metal occurs at 25 GPa. Band features close to the Fermi level are found to be advantageous for high values of thermopower. Our transport calculations also find pressure-enhanced electrical conductivities, high values of thermopower (up to a few hundred μV/K), and significant values of the thermoelectric figure of merit (above 0.10 for high pressure and even up to 0.65 at 25 GPa) over a wide temperature range. Our study supplies a new route to improve the thermoelectric performance of MoS_2 and of other transition metal dichalcogenides by applying hydrostatic pressure.

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