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Thermal Transport Properties of Transition Metal Dichalcogenide Monolayers HALUK YAPICIOGLU, Anadolu University, ARASH MOBARAKI, Bilkent University, ALI KANDEMIR, Izmir Institute of Technology, TAHIR CAGIN, Texas A and M University, OGUZ GULSEREN, Bilkent University, CEM SEVIK, Anadolu University — The characterization of thermal transport in low-dimensional transition metal dichalcogenides (TMDs) is required for their efficient implementation, either for general overheating issues or specific applications in thermoelectric devices. In this study, the lattice thermal conductivities of single-layer MoS_2, $MoSe_2$ WS_2, and WSe_2 are evaluated using classical molecular dynamics simulations. The interactions between atoms are defined by Stillinger-Weber type empirical potentials. In the parameterization of the potentials, a stochastic optimization algorithm, namely particle swarm optimization, is utilized. For the materials considered in this study, the final parameter sets produce quite consistent results with density functional theory in terms of lattice parameters, bond distances, elastic constants, and vibrational properties. The predicted thermal properties of all materials are in very good agreement with earlier first principles calculations.

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