Machine Learning Assisted Prediction of Aperiodic Superlattice Structures with Ultralow Lattice Thermal Conductivity for NASA's Radioisotope Thermoelectric Generators

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Radioisotope thermoelectric generator (RTG) has been the only viable power source for several of NASA's deep space missions. However, the poor energy conversion efficiency of thermoelectric materials greatly limits the efficiency of RTGs, which further limits various aspects of RTG-powered missions. Minimizing the lattice thermal conductivity has been sought for as an effective strategy for developing thermoelectric materials with a high figure of merit. Phonon localization in aperiodic superlattice (ASL) structures has been found to be very effective for designing low lattice thermal conductivity multilayer structures. In fact, ASL structures exhibit much lower lattice thermal conductivity than their periodic counterparts, i.e., periodic superlattice (PSL) due to the localization of coherent phonons. However, finding the optimal configuration, i.e., layer thickness distribution and order of the thicknesses, to achieve the lowest possible thermal conductivity has been a daunting task. This primarily arises from a lack of knowledge of how ASL configuration affects the behavior of coherent phonon transport and localization. In this work, we have identified several structural parameters that are strongly correlated with the lattice thermal conductivity of the ASL structures using classical molecular dynamics simulations. We have revealed that they affect the coherent phonon band structure and thus transmission significantly. Moreover, we have found that using physics-aided machine learning, which considers both configuration and the structural parameters identified through this work altogether, can predict the thermal conductivity of ASLs more accurately and efficiently. In addition, we found that doping a binary ASL with impurities can reduce thermal conductivity significantly, especially when the impurity atom has an atomic mass lower or higher than both of the two base elements. Our findings will be important for developing highly efficient thermoelectric materials for RTGs.