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## Developing a machine learning tool to optimize thermal transport

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## **ABSTRACT**

One of the largest problems facing the world today is energy. Not only does much of the world use non-renewable energy, but the majority of that energy is lost as waste heat. One area of study that aims to solve this problem is thermoelectrics. Thermoelectrics encompasses a wide range of methods and materials but this paper will only cover superlattice structures and how they can be used to convert waste heat into electrical energy. There arises a problem in this of what the best structure is. The method used to optimize the superlattice structure is a genetic algorithm. This method mimics natural selection by first, creating a set of structures (initial population), calculating the thermal conductivity for those structures (evaluating fitness), and selecting the best structures to create the next generation (selection), and finally, performing crossover and mutation on the previously selected structures to create the new population (crossover and mutation). The results of this method show a significant improvement in minimizing thermal conductivity from the initial to the final structures, with the final structures showing a thermal conductivity approximately one-fourth that of the initial structures. Not only is there an improvement in thermal conductivity, but as the optimization process goes on, one can see the spread of results for each generation getting smaller. This method will prove to optimize thermoelectric materials, which can be further implemented in real products to reduce waste heat.

## **KEYWORDS**

Thermoelectric, genetic algorithm, superlattice, crossover, mutation