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Designing nanostructured mixed Heusler systems for improved thermoelectrics VANCHO KOCEVSKI, CHRIS WOLVERTON, Material Science and Engineering Department, Northwestern University — The search for new and more efficient thermoelectric materials has been largely focused on the improvement of the thermoelectric figure of merit by forming nanostructures in a host matrix. Special interest has been directed at the Heusler compounds, especially due to their favorable electrical properties and the possibility of lowering their thermal conductivity via nanostructuring. Aiming to guide future experiments, we predict the possibility of forming nanostructured systems between full and half Heusler host matrices, and other Heusler compounds using density functional theory calculations. Our prediction is based on estimating the solvus between two Heusler compounds, the matrix and the nanostructured compound, using their mixing energy and considering the pairs within a mixing energy interval that favors nanostructuring. Screening the Heusler pairs using this approach gave 25 matrix/nanostructured compound pairs that have not been previously considered as nanostructured thermoelectrics. In addition, based on the mixing energies we argue that different types of Heusler compounds, e.g. half and full Heusler, would favor formation of stable interfaces with low intermixing between the phases, and Heusler compounds of the same type would form nanocomposites or solid solutions.

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