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**On Seebeck Coefficients in Nanostrucutred Graphene and Molecules** CHANGWOOK JEONG, MARK LUNDSTROM, Purdue University — Recently, there has been great interest in enhancing the Seebeck coefficient by a variety of techniques such as nanostructuring graphene, and appropriately engineering molecules. This raises the question of how much the Seebeck coefficient can be changed through bandstructure engineering. In this paper, we use a simple one level model for thermoelectrics as a baseline for comparison and show that within a single particle framework, all materials display a Seebeck coefficient that is close to the single level model. Under some conditions, much lower values can be obtained, but it does not appear possible within this framework to achieve substantially larger values. The conclusion is that familiar thermoelectric concepts apply to novel materials such as nanostructured graphene and to molecules and that to obtain substantially larger Seebeck coefficients, we will need to go beyond the single particle, independent electron picture and explore strongly correlated materials , electron-phonon coupling, etc.

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