

Thermoelectric properties of molecular junctions with Fano resonances

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I present a series of calculations and simulations on the thermoelectric properties of molecular and atomic junctions. I show how the presence of Fano resonances and other types of resonances enhance the thermoelectric coefficient and the figure of merit. I discuss the effect of various factors such as the molecular structure, the coupling between the molecule and the leads, gate voltages and bias voltages. These results are used to derive general trends in the thermoelectric response of atomic and molecular junctions and to predict the most favourable combination of factors that increase the thermoelectric performance.