

Enhanced Figure of Merit in Molecular Junctions

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ABSTRACT

In order to convert the wasted heat into useful energy, thermoelectric devices are designed to maximize the figure of merit ZT defined as the ratio of the electric and thermal conductivity times the Seebeck coefficient. However, most of devices suffer from the small value of ZT ($ZT < 1$) and use mostly doped semiconductors. Here, we show that molecular junctions can have a higher value of ZT , paving the way for efficient thermoelectric devices. Using the density functional theory combined with non-equilibrium Green's function, we calculate, in linear response regime and Landauer-Buttiker approach, the figure of merit for different types of junctions. The molecular junctions have values of $ZT > 3$ and can be increased by an order of magnitude by different physical and chemical means.

References

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