Impact of increasing the number of molecules in thermopower properties of C_{20} molecule

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Received: 25.06.2016 Final revised: 26.06.2018 Accepted: 22.10.2018

Abstract

In this research, thermopower properties of C_{20} fullerene molecule and the effect of increasing the number of molecule were investigated using density functional theory and equilibrium Green's function formalism in linear response regime. We consider three different configurations: Au-C_{20}-Au, Au-$(C_{20})_2$-Au and Au-$(C_{20})_3$-Au. The calculation shows that increasing the number of C_{20} fullerene molecules in the device increases the molecular thermopower. In addition, the signs of the thermopower are length dependent and can be positive (p type) or negative (n type) for different numbers of C_{20} fullerene molecules. Thermopower increases the figure of merit in the system and leads to more efficient thermoelectric device.

Keywords: Thermopower, C_{20} fullerene, Density functional theory, Equilibrium Green's function

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