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Power-efficiency trade-off due to density of states (DOS) distortion in a molecular thermoelectric system PRIYANKA DESOUZA, Department of Energy Science and Engineering, IIT Bombay, Powai, Mumbai-400076, India, BHASKARAN MURALIDHARAN, Department of Electrical Engineering, IIT Bombay, Powai, Mumbai-400076, India — The issue of how a distortion in the electronic DOS affects nanoscale thermoelectric performance is addressed within an "electrical engineering" perspective. This view point is based on the direct evaluation of the overall efficiency and power from device current-voltage characteristics and gives a more complete picture of the thermoelectric performance in comparison to the traditional "figure of merit" based material science approach. We use representative examples from molecular conduction to study the trade-off between maximum efficiency and the maximum power generated within the set up. The trade-off is maximum for the well known example of a sharply resonant molecular level which represents the ultimate distortion in the electronic density of states. As the distortion is reduced via contact induced broadening, we obtain a smaller trade-off between maximum power and efficiency. We then present the effects of self consistent charging, contact induced asymmetry and the HOMO-LUMO gap on the thermoelectric performance. In all cases we compare our non-equilibrium calculations with zT calculations, and our results depict that zT is not the sole metric for the assessment of nanoscale thermoelectric performance.

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