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Designing π-stacked molecular structures to be thermal insulators but electric conductors[1] GEDIMINAS KIRSANSKAS, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, QIAN LI, Nano-Science Center and Department of Chemistry, University of Copenhagen, MARTIN LEIJNSE, Solid State Physics and Nanometer Structure Consortium, Lund University, GEMMA SOLOMON, Nano-Science Center and Department of Chemistry, University of Copenhagen, KARSTEN FLENSBERG, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — We show that π-stacked molecular structures in transport junctions can be designed to have a reduced thermal phonon conductance, while maintaining a high electric conductivity. The relevant contribution to the phonon thermal conductance, up to room temperature, comes from the center of mass motion of the molecules. Therefore, we propose a molecular design consisting of two large masses coupled to each other and to the leads. By having a small coupling (spring constant) between the masses, it is possible to reduce the phonon thermal conductance. This can be achieved by a π-stacking of the molecules. For the proposed model, the effects of mass' asymmetry, coupling asymmetry, and coupling strength are also examined. The resulting heat conductance is compared with the situation when the molecule is modeled as a single mass. The effective coupling strengths (spring constants) for the simplified model are extracted from density functional theory calculations.

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