

Abstract Submitted
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Thermoelectric transport through single molecule junctions MARIUS ERNST BUERKLE, Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan, THOMAS HELLMUTH, Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany, FABIAN PAULY, Department of Physics, University of Konstanz, 78457 Konstanz, Germany, YOSHIHIRO ASAI, Nanosystem Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan — The charge and heat transport properties of single multilayered cyclophane stacks connected to gold electrodes are calculated in the framework of ab initio electronic structure calculations combined with non-equilibrium greens function techniques. The heat transport include both the electronic and phononic contribution, which allows a fully ab initio determination of the thermoelectric transport properties. We investigate the influence of the molecular length and of the molecule-electrode binding motif on the electron and phonon transport characteristics. We find that the power factor is limited due to the fact that the Wiedeman-Franz law remains approximate valid due to the strong off-resonant electron transport. On the other hand the large phonon mismatch between the molecule and the gold electrodes leads to a suppression of the phonon thermal conductance.

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