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Quantum Resonance Effects to Thermoelectric Property of Organometallic Molecular Materials HISAO NAKAMURA, National Institute of Advanced Industrial Science and Technology (AIST) — Superior long-range electric transport has been observed in several organometallic wires and films. Here, we propose use of organometallic molecules for thermoelectric materials by focusing on the overlapping resonance effect, which enables long-range coherent tunneling and enhancement of Seebeck coefficient. We examine the possibility of high thermoelectric figure of merit (ZT) by controlling the quantum resonance based on first principles transport calculations of electron and phonon. [1] We found distinct length and temperature dependences of ZT from those of inorganic bulk materials or organic molecules. We will present an alternative approach to obtain high ZT by using organometallic molecular materials.

[1] H. Nakamura, T. Ohto, T. Ishida, and Y. Asai, *J. Am. Chem. Soc.* DOI: 10.1021/ja407662m

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