Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Superior Long range Electric Transport of Organometallic Wire via Stepping Stone mechanism and First Principles Study of Length dependence of Thermoelectric Effects HISAO NAKAMURA, TAKAO ISHIDA, YOSHIHIRO ASAI, The National Institute of Advanced Industrial Science and Technology (AIST) — We revealed the role of metal centers for superior long-range electric transport in organometallic-complex wires via stepping stone mechanism, which is recently proposed in Ref. 1]. We also found that the transport properties of organometallic molecular wire have some advantages to create thermoelectric devices, such as phonon mismatching effect, superior long range transport, and quantum interferences of conducting orbitals. We analyzed the length dependence and metal species dependence of the figure of merit (ZT) with including phonon thermal conductivity based on the first principles calculations. [1] K. Terada, H. Nakamura, K. Kanaizuka, M. Haga, Y. Asai, and T. Ishida, ACS Nano, 6, 1988-1999 (2011).

Hisao Nakamura
The National Institute of Advanced
Industrial Science and Technology (AIST)

Date submitted: 27 Nov 2012 Electronic form version 1.4