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First-Principles Study on Thermoelectric Properties of Carbon Nanotubes JOUNGHEE LEE, EUI-SUP LEE, YONG-HYUN KIM, KAIST — Carbon nanotubes (CNTs) have attracted much attention because of their extraordinary material properties such as strong mechanical strength, chirality- and diameter-dependent electronic structure, and high thermal conductivity. As an electronic property, the Seebeck coefficient should also sensitively depend on the charility and diameter of CNTs. In this work, we propose a way to calculate an intrinsic Seebeck coefficient of one-dimensional CNT systems based on coherent electron transport within first-principle calculations and Landauer formulation. We will also estimate a contribution from diffusive transport, comparing to experimental results. The calculated maximum Seebeck coefficient is 0.13 mV/K for (9,9) metallic CNTs, while it is 0.8 mV/K for (10,8) semiconducting CNTs with similar diameter. When the diameter is smaller, the Seebeck coefficient of semiconducting CNTs can be as big as 1.3 mV/K with appropriate doping level.

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