# Large-scale simulation on electron transport of carbon-nanotube composites for reducing environmental loads


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## Abstract

Carbon-nanotube copper (CNT-Cu) composite possesses the following desirable properties: high conductivity comparable to that of Cu, lower temperature-dependence of the conductivity than that of Cu, and 100-times higher ampacity than that of Cu. These significant properties, however, has not been fully understood so far. In order to understand the origin of these properties, we have searched atomic structures of the CNT-Cu composite for high conductivity and studied the effect of atomic vibration on the conductivity. For this purpose, we investigated the transport properties of CNT-Cu composites through a large-scale simulation using a non-equilibrium Green's function method based on density functional theory. In a CNT-wire wrapped uniformly by Cu, high conductivity, to which states of the CNT contribute, is observed. This contribution of CNT states is due to the energy shift of CNT band caused by wrapping Cu. Our findings show that the composites of zigzag-type CNT have much more potential for high conductivity than those of armchair-type CNT. In addition, while in the CNT-Cu wire, Cu atoms oscillate by applied heat, the atomic vibration of Cu in bundled CNT is expected to be suppressed.



**Keywords:** Carbon nanotube, Composite material, First-principles density functional theory, Non-equilibrium Green's function, current-induced force