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First-principles study of charge transfer doping and electronic transport in single-walled carbon nanotubes¹ XIANGGUO LI, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, Florida 32611, USA — It is well known that charge transfer doping can greatly enhance the conductivity in single-walled carbon nanotube thin films. Recent experiments showed that the tube-tube contact resistance dominates the impedance in the films. To understand effects of doping on the tube-tube contact, we studied the tube-tube distance changes and electron transport properties upon doping (K and Br) using first-principles calculations. Our results suggest that the effect of doping on the tube-tube distance depends not only on the type of dopants but also on the electronic properties of the carbon nanotubes.

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