Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information to: "The loaded amount and arrangement of iodine chains affect the interfacial thermal transport of carbon nanotube: A molecular dynamics study"

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I. Thermal conductance of CNT with variety overlap length

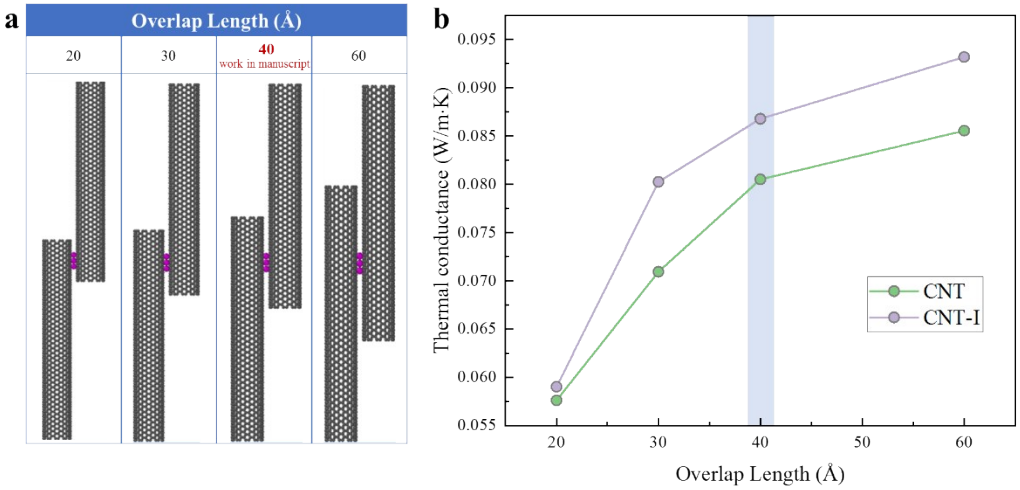

Fig. S1 Thermal conductance of CNT with or without iodine chains in overlap length of 20, 30, 40 and 60 Å. a) the scheme of calculation model, b) the thermal conductance results.

As shown in the Fig. S1, it illustrates the variation of thermal conductance of CNT interface with change in CNT overlap length. With the increase of the overlap length, the heat transfer of the CNT interface shows an increasing trend, and it further improve after iodine chain loaded.

For the overlap length of 20 Å, the iodine chain is close to the boundary of the

overlap region, and the strengthening effect is interfered. For 40 and 60 Å, the overlap region is longer, and the iodine chain can only react with a part of carbon atoms. The overlap length of 30 Å may be closer to the optimal overlap length when one on each side of the loaded iodine chain. A longer overlap area is beneficial to the thermal transfer between the tubes, and at the same time, a suitable iodine chain loading amount can have a greater strengthening effect.

II. Heat transfer and mechanism of CNT-Cu

Fig. S2 illustrates the CNT-Cu calculation model and its thermal conductance, which is compared with the pristine CNT and CNT-I of this work. The CNT overlap length of all of these cases are set to 40 Å. In order to compare with the CNT- I3- case, each cluster contain 3 copper atoms. The structure of Cu cluster is source from Doye and Wales' work[1] with the lattice constant 3.596 Å[2]. For the atoms interact force of CNT-Cu, The Modified Embedded-Atom Method (MEAM)[3] force field is used to describe the atom interaction of Cu atoms, the force between Cu and CNT have used Lennard-Jones potential, and the C atoms in CNT also described by Adaptive Intermolecular Reactive Empirical Bond Order (Airebo) potential. The thermal conductance was calculated by the Non-equilibrium molecular dynamics (Fig.S2), and the Vibration Density of States(VDOS) of carbon atoms in overlap area of the two CNT and the Cu clusters shown in the Fig.S3.

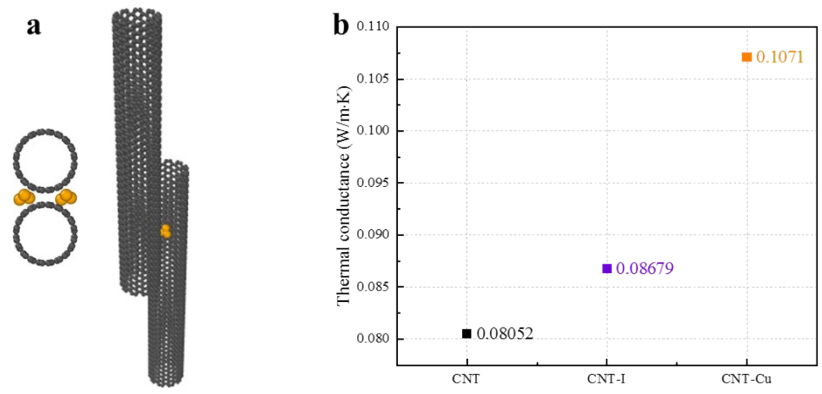

Fig. S2 The thermal conductance of pristine CNT, CNT-Cu. (a) the scheme of CNT loaded copper cluster. (b) the thermal conductance results.

From the Fig.S2, it can be realized that the thermal conductance increased after iodine chains and copper clusters loaded, and the Cu cluster with 3 atoms is more effective for interfacial heat transfer enhancement. VDOS reveal internal mechanisms in simply explanation form(Fig.S3). The surface of the spherical copper clusters contains more abundant low-frequency phonon modes[4], which strengthens the induction of low-frequency phonon modes. After loading the copper nanoclusters, the low-frequency phonon peaks of the carbon atoms in the overlapping part have been strengthened, which around 13 and 20 THz, compared with before loading. The excitation of a large number of low-frequency phonons is the main factor for the copper clusters to strengthen the carbon nanotubes.

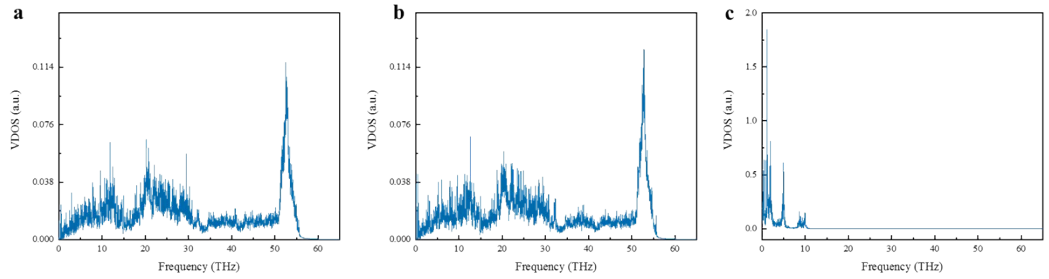

Fig. S3 The vibration density of states of C_{hot} (a), C_{cold} (b) and copper cluster (c).

Reference

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