Supporting Information

Can graphene improve the thermal conductivity of copper nanofluids?

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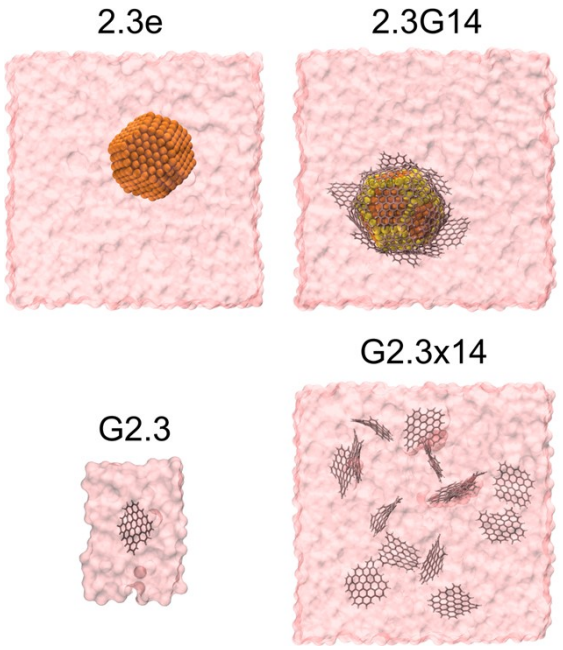

Figure S1 Simulation models to evaluate the contribution of each nanomaterial to the thermal conductivity of the Cu-Ar and Cu capped by graphene (Cu@G)-Ar nanofluids.

Table S1 Summary of the dimensions of the studied systems and their atomic composition.

Model	Box side length (Å)	Cu atoms	C atoms	H atoms	Ar atoms
15	55.3×52.5×46.8	201	-	-	3343
23	62.9×58.8×62.08	586	-	-	4720
31	70.6×65.1×68.5	1289	-	-	6357
40	78.3×71.4×76.9	2406	-	-	8255
6.1	101.1×90.2×69.7	9201	-	-	15443
15G14	72.0×66.2×62.1	201	420	196	5954
23G14	71.6×74.6×72.22	586	812	280	7440
31G14	84.0×79.7×84.9	1289	1540	392	10451
40G14	90.1×85.0×96.4	2406	2212	476	13132
6.1G14	109.2×107.1×115.3	9201	5068	728	21366
23G2	73.1×75.6×73.8	586	828	112	7440
23G36	74.6×77.0×75.6	586	792	430	7440
23G14b	81.8×80.0×76.72	586	1624	560	9348
23G14t	88.1×82.3×88.1	586	2436	840	11251
23G14tp	92.3×91.3×90.6	586	2436	840	11227
23x15	106.7×95.8×104.1	8790	-	-	15443
23G14x15	113.4×105.8×119.3	8790	12180	4200	21366
graphene	51.2×50.3×43.9	-	1008	-	2049
bilayer graphene	51.1×50.1×45.9	-	2016	-	2047
trilayer graphene	49.6×50.6×46.7	-	3024	-	1946

Table S2 Lennard-Jones parameters for the interactions between the atoms of the NPs and the Ar fluid. The Cu-Ar parameters were reported by Lv *et al.*[1] while the C-Ar, H-Ar and Ar-Ar by Fraenkel *et al.*[2]

	ε (eV)	σ (Å)
Cu — Ar	0.0650071	2.872
C — Ar	0.0043400	3.480
H — Ar	0.0040900	3.208
Ar — Ar	0.0103400	3.400

Table S3 Thermal conductivity (κ) of liquid Ar as a function of the simulation time and size of the simulation box at T=86 K and ρ=1418 km/m^3. When the simulation time varies, the box side length was set to 40×40×40 Å^3. When the box size varies, the simulation time remains constant at 1 ns.

Simulation time (ns)	κ (Wm^{-1}K^{-1})	Box side length (Å)	κ (Wm^{-1}K^{-1})
0.25	0.1318	30×30×30	0.1292
0.50	0.1270	40×40×40	0.1105
0.75	0.1278	50×50×50	0.1322
1.00	0.1311	60×60×60	0.1239

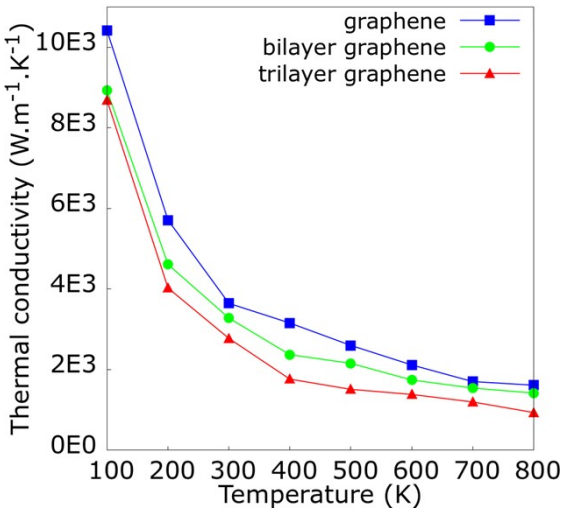

Figure S2 Estimation of thermal conductivity for mono-, bi-, and trilayer infinite graphene, evaluated from 100 to 800 K.

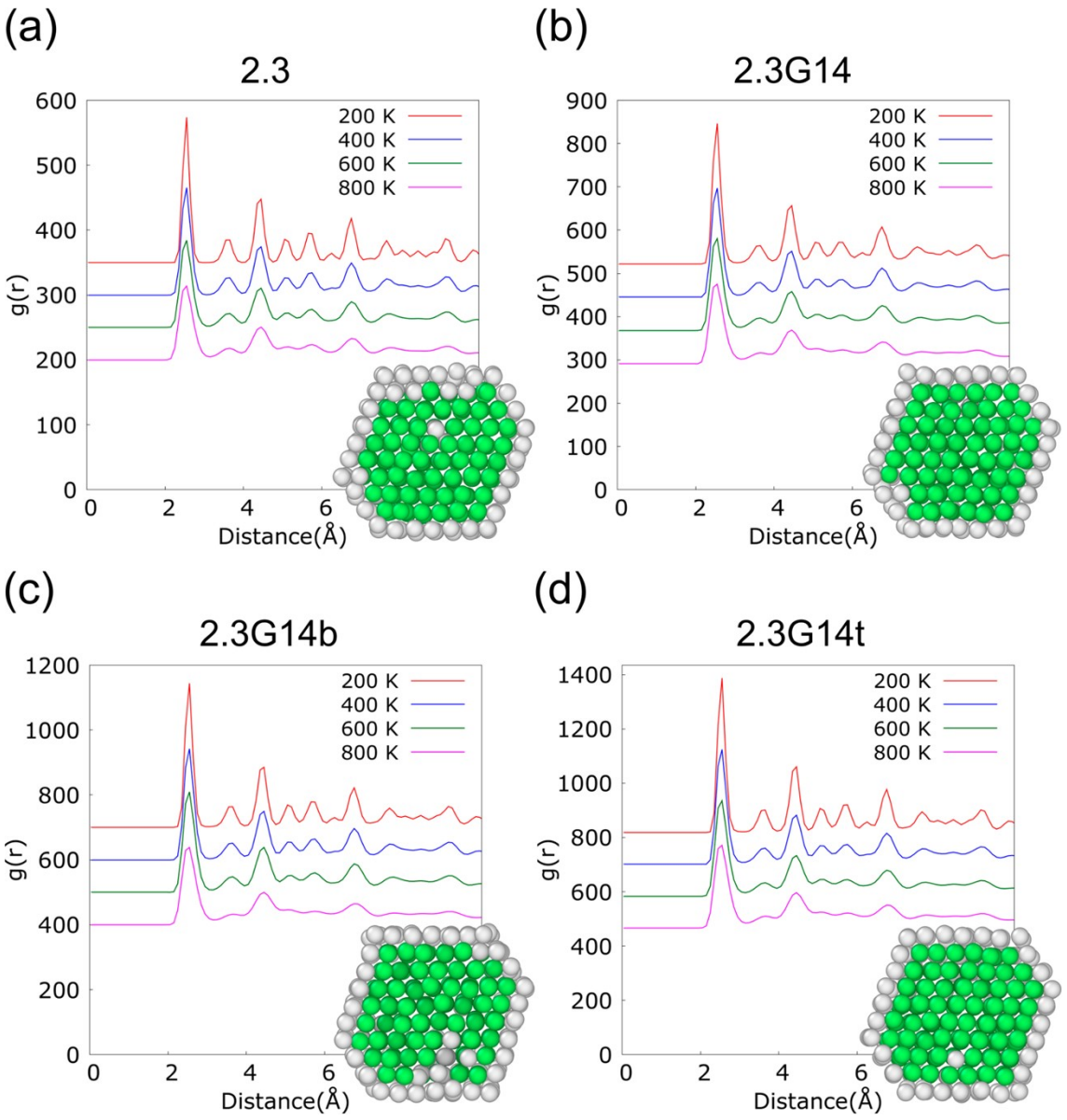

Figure S3 Average Radial Distribution Function (g(r)) and Common Neighbor Analysis (CNA) for the 2.3, 2.3G14, 2.3G14b and 2.3G14t nanofluids during 1 ns of simulation. The green atoms in the CNA represent those that are part of the FCC crystalline structure of the nanoparticle at a given instant at 800 K.

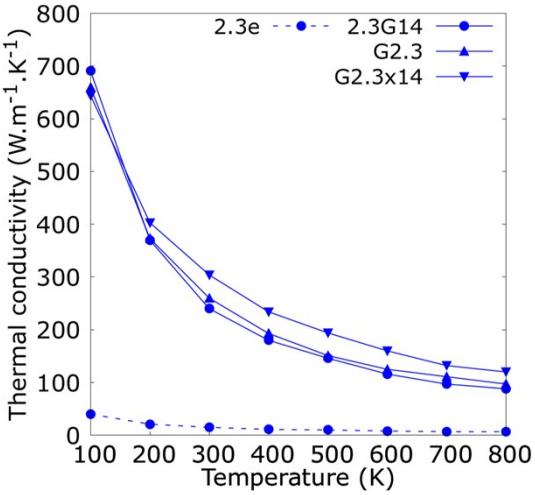

Figure S4 Contribution of each nanomaterial (structured shown in Fig. S1) of the Cu@G NPs in the estimation of thermal conductivity for the nanofluids, and evaluated from 100 to 800 K.

References

1 J. Lv, M. Bai, W. Cui and X. Li, *Nanoscale Res. Lett.*, 2011, **6**, 200.

2 R. Fraenkel, D. Schweke, Y. Haas, F. Molnár, D. Horinek and B. Dick, *J. Phys. Chem. A*, 2000, **104**, 3786–3791.