

## Supporting Information

# Can graphene improve the thermal conductivity of copper nanofluids?

Gabriel J. Olguin-Orellana,<sup>a\*</sup> Germán J. Soldano,<sup>b</sup> María B. Camarada,<sup>c,d</sup> J. Alzate-Morales<sup>a</sup> and Marcelo M. Mariscal<sup>b\*</sup>

<sup>a</sup>. Center for Bioinformatics, Simulation and Modeling (CBSM), Faculty of Engineering, Universidad de Talca, 1 Poniente 1141, Talca, Chile.

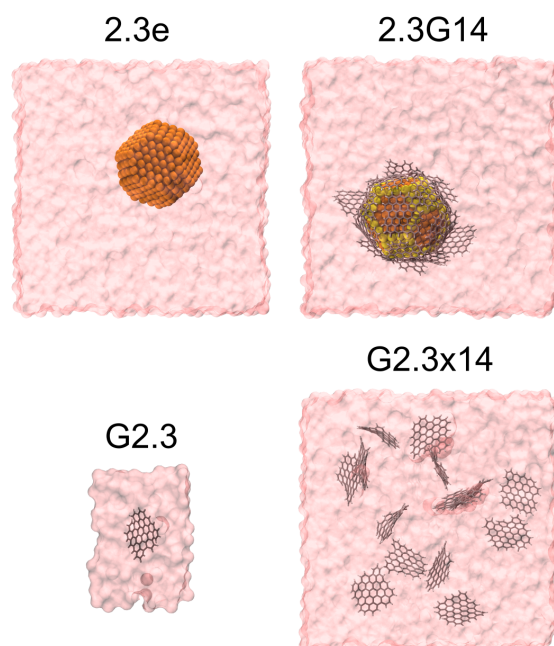
<sup>b</sup>. INFIQC, CONICET, Departamento de Química Teórica y Computacional, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Argentina. E-mail: marcelo.mariscal@unc.edu.ar.

<sup>c</sup>. Laboratorio de Materiales Funcionales, Departamento de Química Inorgánica, Facultad de Química y de Farmacia, Pontificia Universidad Católica de Chile.

<sup>d</sup>. Centro Investigación en Nanotecnología y Materiales Avanzados, CIEN-UC, Pontificia Universidad Católica de Chile, Santiago, Chile.

DOI: 10.1039/x0xx00000x

E-mail: [mbcamara@uc.cl](mailto:mbcamara@uc.cl) / [marcelo.mariscal@unc.edu.ar](mailto:marcelo.mariscal@unc.edu.ar)



**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.

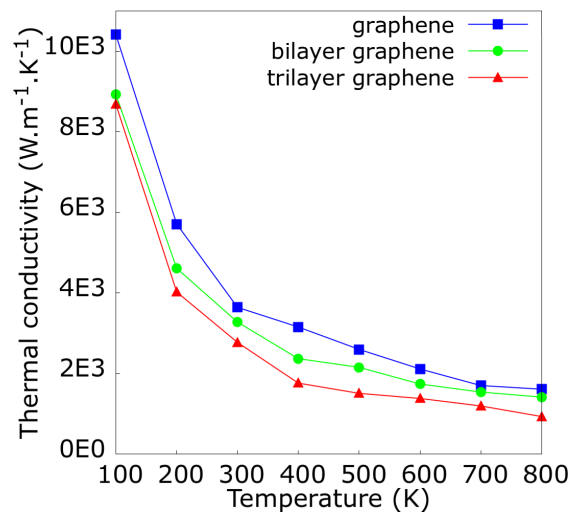
Model	Box side length (Å)	Cu atoms	C atoms	H atoms	Ar atoms
15	55.3×52.5×46.8	201	-	-	3343
23	62.9×58.8×62.08	586	-	-	4720
31	70.6×65.1×68.5	1289	-	-	6357
40	78.3×71.4×76.9	2406	-	-	8255
6.1	101.1×90.2×69.7	9201	-	-	15443
15G14	72.0×66.2×62.1	201	420	196	5954
23G14	71.6×74.6×72.22	586	812	280	7440
31G14	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.*<sup>1</sup> while the C-Ar, H-Ar and Ar-Ar by Fraenkel *et al.*<sup>2</sup>

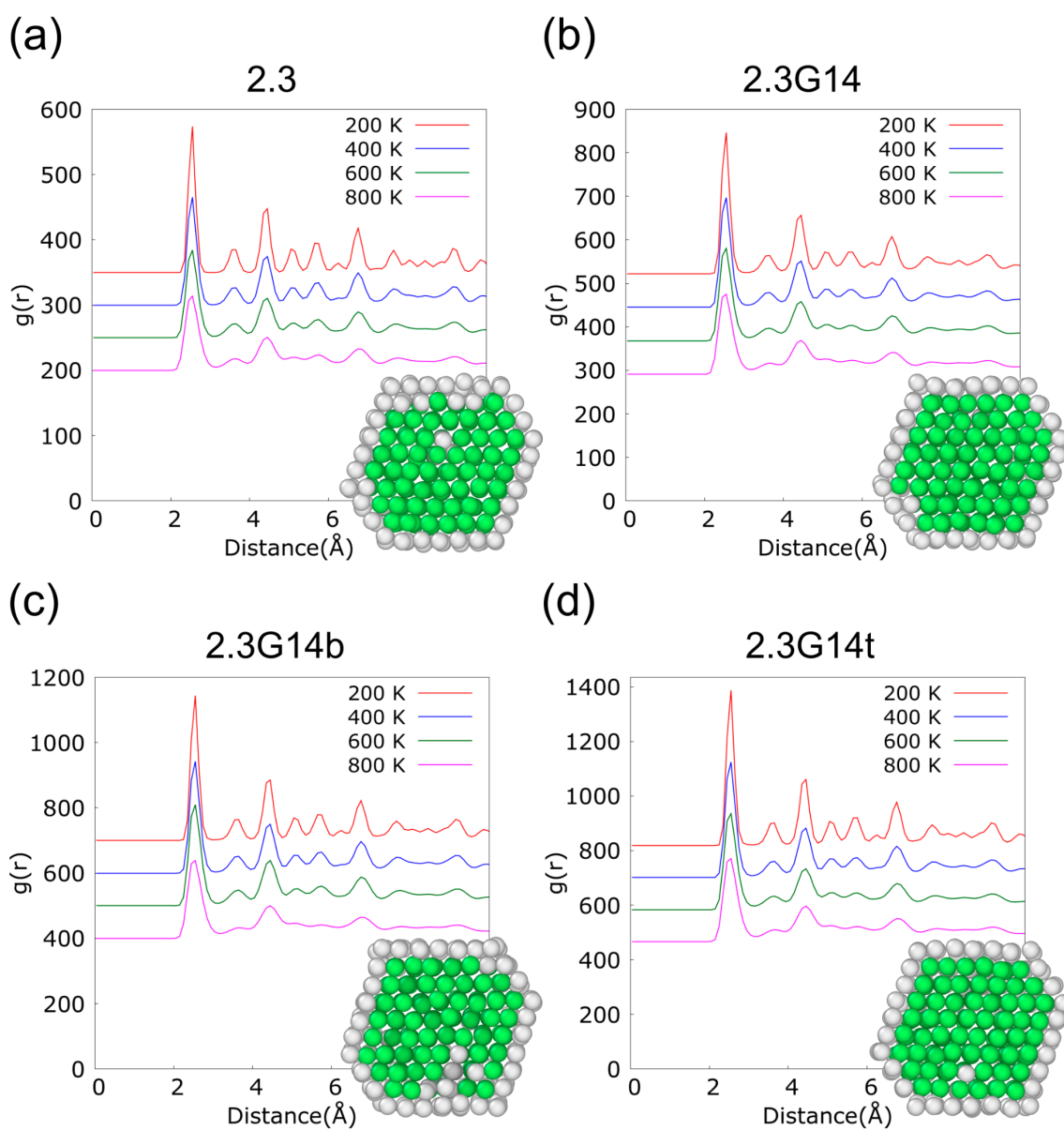
	$\epsilon$ (eV)	$\sigma$ (Å)
Cu — Ar	0.0650071	2.872
C — Ar	0.0043400	3.480
H — Ar	0.0040900	3.208
Ar — Ar	0.0103400	3.400

**Table S3** Thermal conductivity ( $\kappa$ ) of liquid Ar as a function of the simulation time and size of the simulation box at T=86 K and  $\rho=1418 \text{ km/m}^3$ . When the simulation time varies, the box side length was set to  $40 \times 40 \times 40 \text{ \AA}^3$ . When the box size varies, the simulation time remains constant at 1 ns.

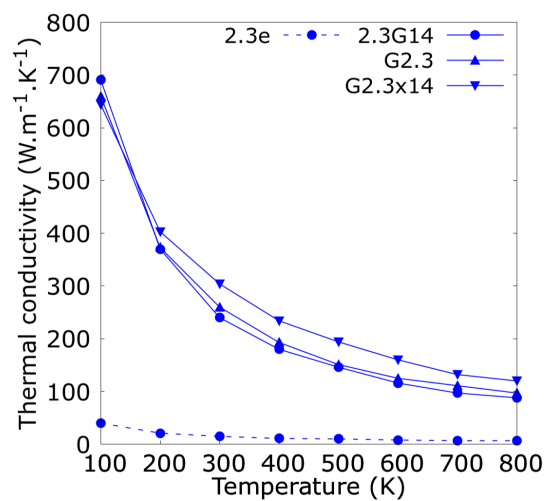
Simulation time (ns)	$\kappa$ ( $\text{Wm}^{-1}\text{K}^{-1}$ )	Box side length (Å)	$\kappa$ ( $\text{Wm}^{-1}\text{K}^{-1}$ )
0.25	0.1318	$30 \times 30 \times 30$	0.1292
0.50	0.1270	$40 \times 40 \times 40$	0.1105
0.75	0.1278	$50 \times 50 \times 50$	0.1322
1.00	0.1311	$60 \times 60 \times 60$	0.1239



**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.