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Correction: Ultra-high thermal conductivities of tetrahedral carbon allotropes with non-simple structures

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Correction for 'Ultra-high thermal conductivities of tetrahedral carbon allotropes with non-simple structures' by Qiang Chen et al., *Phys. Chem. Chem. Phys.*, 2021, DOI: 10.1039/d1cp02347k.

(1) The sentence

"It is found that the thermal conductivities of three carbon allotropes of C₃₂, C₃₆, and C₉₄ with non-simple structure can be as high as 1152.75, 1075.70, and 860.07 W m⁻¹ K⁻¹, respectively, despite a large number of atoms in the primitive cell." beginning on line 5 of the Abstract on page 1 should be written as

"It is found that the thermal conductivity of three carbon allotropes of C₃₂, C₃₆, and C₉₄ with non-simple structures can be as high as 1152.75, 1075.70, and 913.64 W m⁻¹ K⁻¹, respectively, despite the large number of atoms in the primitive cell."

(2) The sentence

"Besides, the thermal conductivity value of C₉₄ is 860.07 W m⁻¹ K⁻¹, which is a little bit smaller than those of C₃₂ and C₃₆." beginning on line 10, page 3, right column, in the Results and discussion subsection 3.2 should be written as

"Besides, the thermal conductivity of C₉₄ is 913.64 W m⁻¹ K⁻¹, which is a little bit smaller than those of C₃₂ and C₃₆."

(3) Fig. 3 should be corrected as shown below:

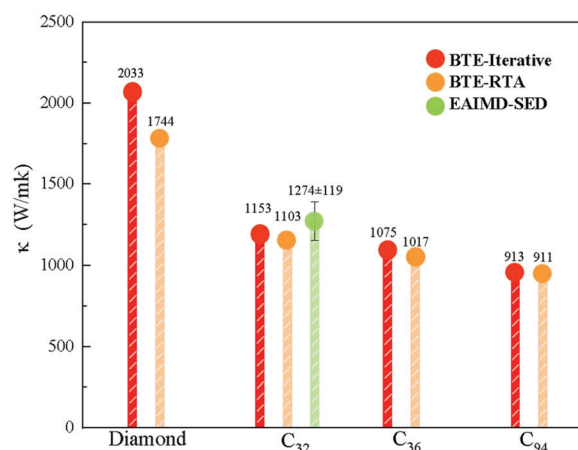


Fig. 3 The comparison of thermal conductivity calculated by different methods.

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(4) The sentence

“As collected in Table 1, the thermal conductivity value of C_{32} is calculated to be $1274 \pm 119 \text{ W m}^{-1} \text{ K}^{-1}$ by fitting the supercell size (Fig. S7 in the ESI†), which is well consistent with the iterative solution of the BTE ($1268 \text{ W m}^{-1} \text{ K}^{-1}$).”

beginning on line 17, page 3, right column, in the Results and discussion subsection 3.2 should be written as

“As collected in Table 1, the thermal conductivity of C_{32} is calculated to be $1274 \pm 119 \text{ W m}^{-1} \text{ K}^{-1}$ by fitting the supercell size (Fig. S7 in the ESI†), which is well consistent with the iterative solution of the BTE ($1153 \text{ W m}^{-1} \text{ K}^{-1}$).”

(5) The sentence

“The results show that C_{32} , C_{36} , and C_{94} possess ultra-high lattice thermal conductivity values, which are 1152.75, 1075.70, and $860.07 \text{ W m}^{-1} \text{ K}^{-1}$, respectively.”

beginning on line 4 of the Conclusions on page 6 should be written as

“The results show that C_{32} , C_{36} , and C_{94} possess ultra-high lattice thermal conductivity values, which are 1152.75, 1075.70, and $913.64 \text{ W m}^{-1} \text{ K}^{-1}$, respectively.”

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

