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Correction: Atomistic QM/MM simulations of the strength of covalent interfaces in carbon nanotube–polymer composites

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Correction for 'Atomistic QM/MM simulations of the strength of covalent interfaces in carbon nanotube–polymer composites' by Jacek R. Gołębowski *et al.*, *Phys. Chem. Chem. Phys.*, 2020, **22**, 12007–12014, DOI: 10.1039/d0cp01841d.

The authors would like to correct a referencing error in the published article and fix a measurement value that was incorrectly copied from the reference.

The changes are in the last paragraph of section 3 on page 12012. The original text reads as follows:

“The experiments of Barber *et al.*¹⁶ demonstrate that the pull-out force is proportional to the embedded surface area of the CNT and recorded the ISS (maximum pullout force over CNT area) of around 50 MPa. For comparison, our simulations give a value of around 1000 MPa, *i.e.*, a factor of 20 larger.”

This should be changed to the following text, where the new reference is added here as ref. 1:

“Earlier experiments by Barber *et al.*¹ demonstrate that the pullout force is proportional to the embedded surface area of the CNT. For carboxyl-functionalised CNTs the maximum ISS is measured to be around 150 MPa.¹⁶ For comparison, our simulations give a value of around 1000 MPa, *i.e.*, an order of magnitude larger.”

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

References

- 1 A. H. Barber, S. R. Cohen and H. D. Wagner, *Appl. Phys. Lett.*, 2003, **82**, 4140.

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