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CORRECTION

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Cite this: Phys. Chem. Chem. Phys., 2025, 27, 2273

Correction: The effect of particle size on the optical and electronic properties of hydrogenated silicon nanoparticles

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DOI: 10.1039/d4cp90219i

rsc.li/pccp

Correction for 'The effect of particle size on the optical and electronic properties of hydrogenated silicon nanoparticles' by Eimear Madden et al., Phys. Chem. Chem. Phys., 2024, 26, 11695-11707, https://doi.org/10.1039/D4CP00119B

The authors would like to update some data reported in Fig. 6. The evGW-BSE oscillator strength value for Si₃₅H₃₆ was taken from a calculation in C_1 rather than one using the D_2 point group used for all other datapoints in the figure. The C_1 and D_2 predicted oscillator strength values differ only slightly, difference 2.5×10^{-3} , however, because of the logarithmic scale this makes a noticeable difference to the figure. The corrected Fig. 6 is presented below.

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

Correction

0 ---- Sum within 0.5 eV, TDDFT --★-- Sum within 0.2 eV, TDDFT ---- Lowest excitation, TDDFT Lowest excitation, evGW-BSE Log(Oscillator Strength) -5

Fig. 6 Log of the predicted oscillator strengths of various excitations of SiNPs. The blue circles represent the sum of the oscillator strengths for the excitation energies which lie within 0.5 eV of the lowest excitation for each SiNP, calculated using TDDFT. The grey stars represent the sum of the oscillator strengths for the excitations which lie within 0.2 eV of the lowest excitation for each SiNP, calculated using TDDFT. The green squares represent the oscillator strength of the lowest excitation for each SiNP calculated using TDDFT. The orange triangles represent the oscillator strength of the lowest excitation for each SiNP calculated using evGW-BSE. All calculations used the B3LYP functional and the def2-SVP basis-set.

4

6

Radius / Å

8

10

12

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