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CORRECTION

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Correction: Enhancement of CO₂ binding and mechanical properties upon diamine functionalization of M₂(dobpdc) metal-organic frameworks†

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Correction for 'Enhancement of CO_2 binding and mechanical properties upon diamine functionalization of M_2 (dobpdc) metal-organic frameworks' by Jung-Hoon Lee *et al.*, *Chem. Sci.*, 2018, **9**, 5197–5206.

Regrettably, in the original manuscript, an error was made in the calculations of the zero-point energy (ZPE) and thermal energy (TE) of gas-phase CO_2 . After evaluating eqn (9)–(13) in the ESI,† the authors found that the computed ZPE and TE corrections were in error by around 6.4 kJ mol⁻¹ and 1.6 kJ mol⁻¹, respectively. These ZPE and TE contributions alter the predicted CO_2 binding enthalpies (H_B) in Table 2. Please see below an updated Table 2, which includes the updated values for the ZPE and TE corrections and the CO_2 binding enthalpies (H_B).

The conclusions in the original manuscript remain unchanged upon consideration of these modified corrections, and the computed CO_2 binding enthalpies still compare quite well with experiments, within 8 kJ mol⁻¹ in the worst case (Fe) but typically better.

Table 2 A comparison of computed CO₂ binding energies (E_B) and enthalpies (H_B) (in kJ mol⁻¹) in mmen–M₂(dobpdc) (M = Mg, Mn, Fe, Co, Zn) with the experimental values at a CO₂ loading of 2 mmol g^{-1,37} Zero-point energy (ZPE) and thermal energy (TE) corrections of ammonium carbamate and mmen are considered. All ZPE and TE values are computed at 298 K

This work				Poss
$E_{ m B}$	ZPE	TE	$H_{ m B}$	$ ext{Exp} H_{ ext{B}}$
74.7	-9.2	2.7	68.1	71
68.9	-8.6	2.2	62.5	67
56.2	-8.3	2.3	50.3	58
52.4	−7. 7	2.0	46.8	52
62.4	-7.9	2.8	57.3	57
	E _B 74.7 68.9 56.2 52.4	$\begin{array}{c cccc} E_{\rm B} & {\rm ZPE} \\ & & & & \\ 74.7 & & -9.2 \\ 68.9 & & -8.6 \\ 56.2 & & -8.3 \\ 52.4 & & -7.7 \\ \end{array}$	$E_{\rm B}$ ZPE TE 74.7 -9.2 2.7 68.9 -8.6 2.2 56.2 -8.3 2.3 52.4 -7.7 2.0	$E_{\rm B}$ ZPE TE $H_{\rm B}$ 74.7 -9.2 2.7 68.1 68.9 -8.6 2.2 62.5 56.2 -8.3 2.3 50.3 52.4 -7.7 2.0 46.8

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

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 $[\]dagger$ Electronic supplementary information (ESI) available. See DOI: 10.1039/c7sc05217k