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Correction: Enhancement of CO_2 binding and mechanical properties upon diamine functionalization of M_2(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 CO_2 binding energies (E_B) and enthalpies (H_B) (in kJ mol^{-1}) in mmen–M_2(dobpdc) (M = Mg, Mn, Fe, Co, Zn) with the experimental values at a CO_2 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				Exp
	E_B	ZPE	TE	H_B	H_B
Mg	74.7	−9.2	2.7	68.1	71
Mn	68.9	−8.6	2.2	62.5	67
Fe	56.2	−8.3	2.3	50.3	58
Co	52.4	−7.7	2.0	46.8	52
Zn	62.4	−7.9	2.8	57.3	57

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

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† Electronic supplementary information (ESI) available. See DOI: 10.1039/c7sc05217k