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

Jung-Hoon Lee,^{ab} Rebecca L. Siegelman,^{cd} Lorenzo Maserati,^a Tonatihu Rangel,^{ab} Brett A. Helms,^{ad} Jeffrey R. Long^{cde} and Jeffrey B. Neaton^{*abf}

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Correction for 'Enhancement of CO₂ binding and mechanical properties upon diamine functionalization of M₂(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 CO₂. 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 CO₂ 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 CO₂ binding enthalpies (H_B).

The conclusions in the original manuscript remain unchanged upon consideration of these modified corrections, and the computed CO₂ 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				Exp H_B
	E_B	ZPE	TE	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.

^aMolecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA. E-mail: jboneaton@lbl.gov

^bDepartment of Physics, University of California, Berkeley, California 94720, USA

^cDepartment of Chemistry, University of California, Berkeley, California 94720, USA

^dMaterials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

^eDepartment of Chemical and Biomolecular Engineering, University of California, Berkeley, California 94720, USA

^fKavli Energy Nanosciences Institute at Berkeley, Berkeley, California 94720, USA

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