

CORRECTION

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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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