

Cite this: *Chem. Sci.*, 2019, 10, 6736

## Correction: Enhancement of CO<sub>2</sub> binding and mechanical properties upon diamine functionalization of M<sub>2</sub>(dobpdc) metal–organic frameworks†

Jung-Hoon Lee,<sup>ab</sup> Rebecca L. Siegelman,<sup>cd</sup> Lorenzo Maserati,<sup>a</sup> Tonatihu Rangel,<sup>ab</sup> Brett A. Helms,<sup>ad</sup> Jeffrey R. Long<sup>cde</sup> and Jeffrey B. Neaton<sup>\*abf</sup>

DOI: 10.1039/c9sc90145k

www.rsc.org/chemicalscience

Correction for 'Enhancement of CO<sub>2</sub> binding and mechanical properties upon diamine functionalization of M<sub>2</sub>(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<sub>2</sub>. 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<sup>-1</sup> and 1.6 kJ mol<sup>-1</sup>, respectively. These ZPE and TE contributions alter the predicted CO<sub>2</sub> 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<sub>2</sub> binding enthalpies ( $H_B$ ).

The conclusions in the original manuscript remain unchanged upon consideration of these modified corrections, and the computed CO<sub>2</sub> binding enthalpies still compare quite well with experiments, within 8 kJ mol<sup>-1</sup> in the worst case (Fe) but typically better.

**Table 2** A comparison of computed CO<sub>2</sub> binding energies ( $E_B$ ) and enthalpies ( $H_B$ ) (in kJ mol<sup>-1</sup>) in mmen–M<sub>2</sub>(dobpdc) (M = Mg, Mn, Fe, Co, Zn) with the experimental values at a CO<sub>2</sub> loading of 2 mmol g<sup>-1</sup>.<sup>37</sup> 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.

<sup>a</sup>Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA. E-mail: jboneaton@lbl.gov

<sup>b</sup>Department of Physics, University of California, Berkeley, California 94720, USA

<sup>c</sup>Department of Chemistry, University of California, Berkeley, California 94720, USA

<sup>d</sup>Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

<sup>e</sup>Department of Chemical and Biomolecular Engineering, University of California, Berkeley, California 94720, USA

<sup>f</sup>Kavli Energy Nanosciences Institute at Berkeley, Berkeley, California 94720, USA

† Electronic supplementary information (ESI) available. See DOI: 10.1039/c9sc05217k

