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Addition/Correction

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Correction and Addition to "Tuning Metal–Organic Frameworks with Open-Metal Sites and Its Origin for Enhancing CO_2 Affinity by Metal Substitution"

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Supporting Information

The geometries referred to in the paper were based on PBE optimization with the binding energies refined using single-point PBE-D2 on the PBE geometries. In the caption of Figure 1 and Table 1, however, it was incorrectly stated that the results were based on the PBE-D2 geometries. The binding energy for V-MOF-74 was also incorrectly cited to be 47.3 kJ/mol in Table 1, but the correct binding energy is 52.4 kJ/mol.

In addition, we have performed the full PBE-D2 optimizations. The full PBE-D2 optimization shifts the previous single-point PBE-D2 binding energies using the PBE geometries up by approximately 1–3 kJ/mol and shortens the M–OCO distances consistently by 0.1–0.2 Å. These new full PBE-D2 optimizations lead to the CO_2 binding energies that are even closer to the experiments by Caskey et al. (*J. Am. Chem. Soc.* **2008**, *130*, 10870–10871) compared to the PBE-D2//PBE results cited in our original version. We now added a new table in the Supporting Information (Table S5) that compares the PBE and PBE-D2 optimized results.

In summary, the correction and addition described above do not change any of the conclusions presented in the original version but rather strengthen one of our technical points, the validity of PBE-D2 for the MOF-74/CO_2 system.

■ ASSOCIATED CONTENT

Supporting Information

Calculation details, calculated structural parameters, electrostatic energy estimations, DOS analyses for all metals before and after the binding of CO_2, charge densities for showing orbitals interactions, Bayder charge analysis, forward donation analysis, and comparison of the PBE and PBE-D2 optimized results are described. This material is available free of charge via the Internet at http://pubs.acs.org.

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