Supplementary Information (SI) for Digital Discovery.


# Supplementary Information of "Quantum simulation of carbon capture in periodic metal-organic frameworks"

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Table S1: Contribution of the MP2 correlation energy in the active space to the adsorption energy $\Delta E_{\mathrm{AS}}^{\mathrm{MP2corr}}$ of $CO_2$ in Fe-MOF-74 as obtained with active spaces of different sizes. These results were obtained with a kinetic energy cutoff of 420 eV.

| NO occupation threshold | active space $CO_2$ | active space MOF | active space $CO_2$@MOF | $\Delta E$ kJ/mol |
|---|---|---|---|---|
| $10^{-3}$ | (16,28) | (46,74) | (62,102) | -1.06 |
| $10^{-4}$ | (16,62) | (46,158) | (62,220) | 4.54 |
| $10^{-5}$ | (16,126) | (46,324) | (62,453) | 9.05 |
| $10^{-6}$ | (16,222) | (46,591) | (62,819) | 9.55 |
| $10^{-7}$ | (16,364) | (46,998) | (62,1366) | 9.61 |

Table S2: Energy deviations (in kJ/mol) of the full configuration interaction energies for the triplet and quintet states relative to the singlet state, computed within the reduced active spaces of the MOF and $CO_2$@MOF systems. Positive values indicate a higher energy with respect to the singlet.

| Spin state | MOF | $CO_2$@MOF |
|---|---|---|
| Triplet | 5.53 | 2.81 |
| Quintet | 26.8 | 124 |