



Correction to: The effect of atomic point charges on adsorption isotherms of CO₂ and water in metal organic frameworks

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Correction to: Adsorption (2020) 26:663–685
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Recently, we presented a detailed and systematic molecular simulation study of the effect of point charges on adsorption of carbon dioxide and water in a series of typical MOF materials [1]. Unfortunately, we have since detected a mistake in one of the input files pertaining to water adsorption isotherm simulations—concretely, the structure of the water molecule was modelled as linear instead of obeying the correct H-O-H angle of 109.47° for the SPC/E model [2]. As we later found out, this led to a significant underestimation of the amount adsorbed in all water isotherms reported in our original paper, although the relative differences between isotherms obtained using different charge sets are qualitatively the same. We have repeated all the water adsorption simulations, and report the new results here in graphical format. With the exception of a few minor statements, which we also

correct below, the conclusions of the original work remain unchanged. The new set of atom and molecule files needed to run the GCMC simulations have been made openly available from the University of Strathclyde Knowledge Base at: <https://doi.org/10.15129/1ff38b00-b1ef-47a0-a354-82ee2167b772>

2 Results and discussion

Below we present a new set of figures reporting CO₂ and water adsorption isotherms in each of the MOFs studied in our original work. The same figure numbers as in the original paper were retained. We also report some statements that require corrections from the original discussion.

3.1 IRMOF-1

The original article can be found online at <https://doi.org/10.1007/s10450-019-00187-2>.

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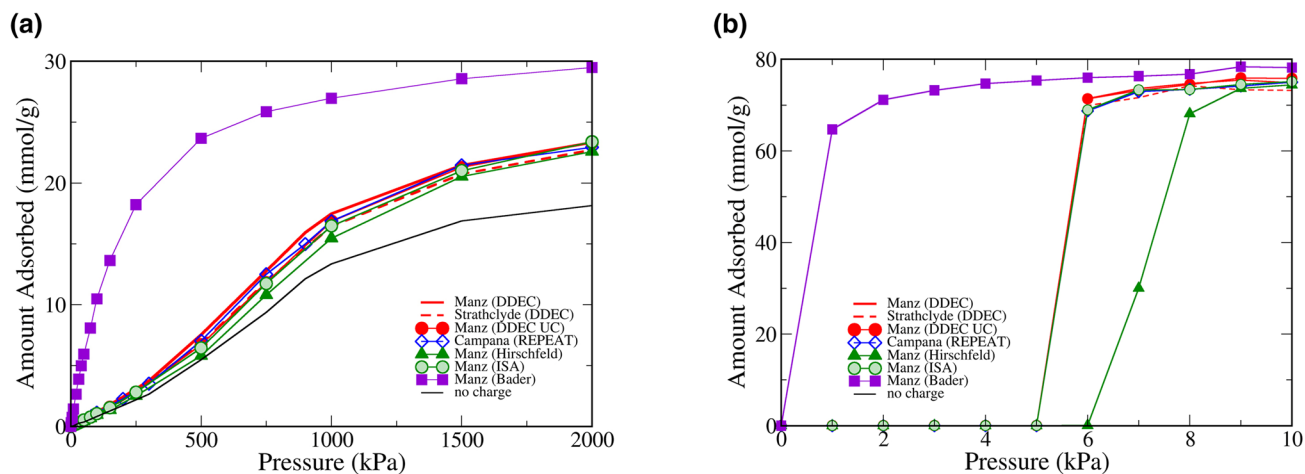


Fig. 2 Adsorption isotherms of: **a** CO_2 ; **b** water in IRMOF-1 at 298 K using point charge sets obtained by periodic methods. Isotherms calculated without any framework charges are shown as a black line

(too low to be visible in the water plot). Error bars are the size of the symbols used

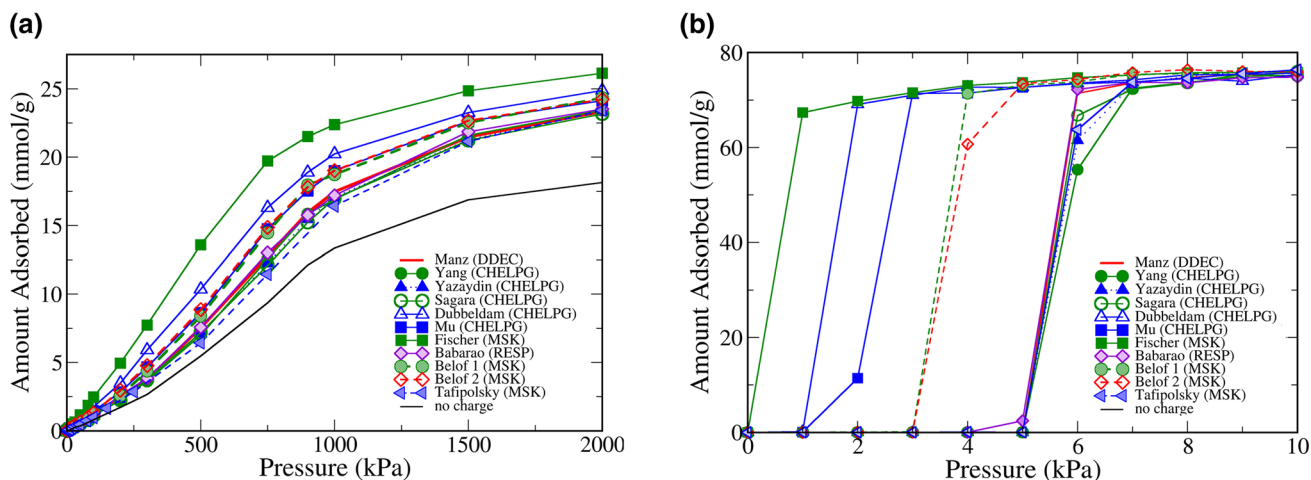


Fig. 3 Adsorption isotherms of: **a** CO_2 ; **b** water in IRMOF-1 at 298 K comparing DDEC point charges (thick red line) to charges obtained from QM cluster calculations. The charge calculation method for each set is reported in the legend. Isotherms calculated without any frame-

work charges are shown as a black line (too low to be visible in the water plot). Error bars are the size of the symbols used (Color figure online)

3.2 MIL-47

The last sentence beginning in page 673 of the original paper [1], which reads as:

“These differences are already statistically significant for CO_2 and are further amplified in the water isotherms (Figure 6b), with the Mulliken charge set now showing a somewhat larger difference relative to the reference case.”

should be replaced with:

“These differences are already statistically significant for CO_2 and are further amplified in the water isotherms (Figure 6b), with three of the charge sets now showing a somewhat larger difference relative to the reference case.”

3.3 UiO-66

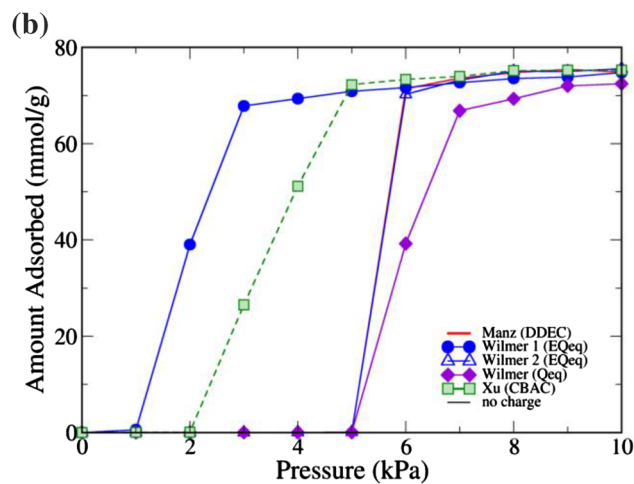
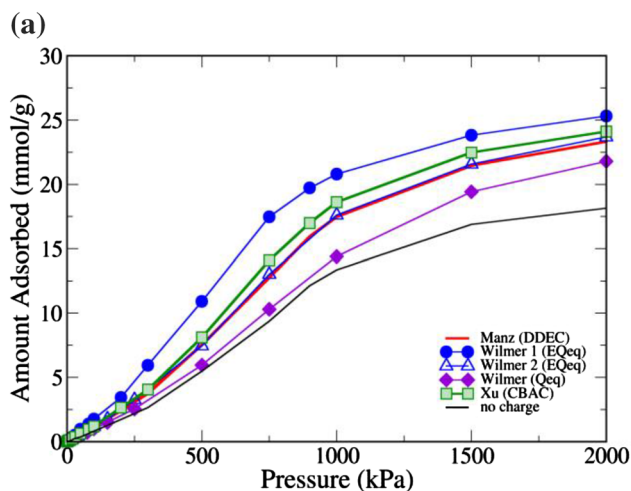


Fig. 5 Adsorption isotherms of: **a** CO₂; **b** water in IRMOF-1 at 298 K comparing DDEC point charges to charges obtained by semi-empirical approaches. Isotherms calculated without any framework charges

are shown as a black line (too low to be visible in the water plot). Error bars are the size of the symbols used

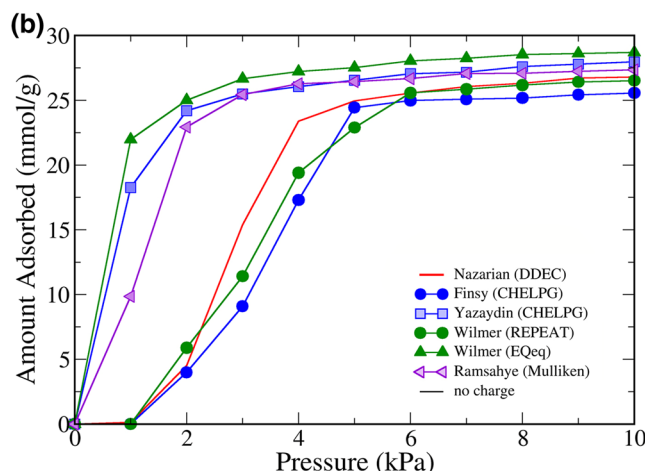
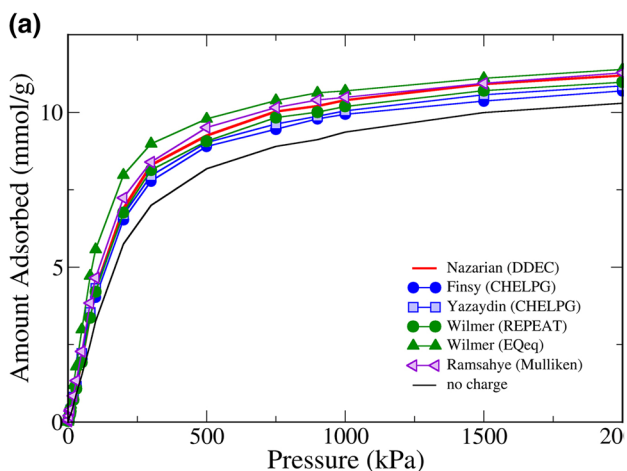


Fig. 7 Adsorption isotherms of: **a** CO₂; **b** water in MIL-47 at 298 K using different point charge sets for the framework atoms. Isotherms calculated without any framework charges are shown as a black line

(too low to be visible in the water plot). Error bars are the size of the symbols used

3.4 CuBTC

The second sentence beginning in page 678 of the original paper [1]:

“The QM cluster-based isotherms show a much more significant degree of variability, with one of the charge sets leading to a two-fold decrease in the pressure at the isotherm inflection point (from ~ 600 to ~ 1250 kPa).”

should be replaced by:

“The QM cluster-based isotherms show a much more significant degree of variability, with two of the charge sets leading to a two-fold decrease in the pressure at the isotherm inflection point (from ~ 3 to ~ 1.5 kPa).”

The fourth and fifth sentences of the second paragraph of page 678 of the original paper [1]:

“The Liu1, Yazaydin2 and Yang sets show almost identical slopes and all have Cu charges around + 1.1; the Babarao, Fischer and Liu2 sets have slightly lower slopes and Cu charges around + 1.05; finally, the periodic sets of Nazarian, Wilmer and Zang have the smallest slopes and Cu charges around + 0.9. The correlation is not perfect, however, with the CBAC, Yazaydin1 and EQeq sets showing steep slopes and relatively low Cu charges.”

should be replaced by:

“There follows a large group of isotherms with relatively high slopes and Cu charges between + 1 and + 1.1; finally,

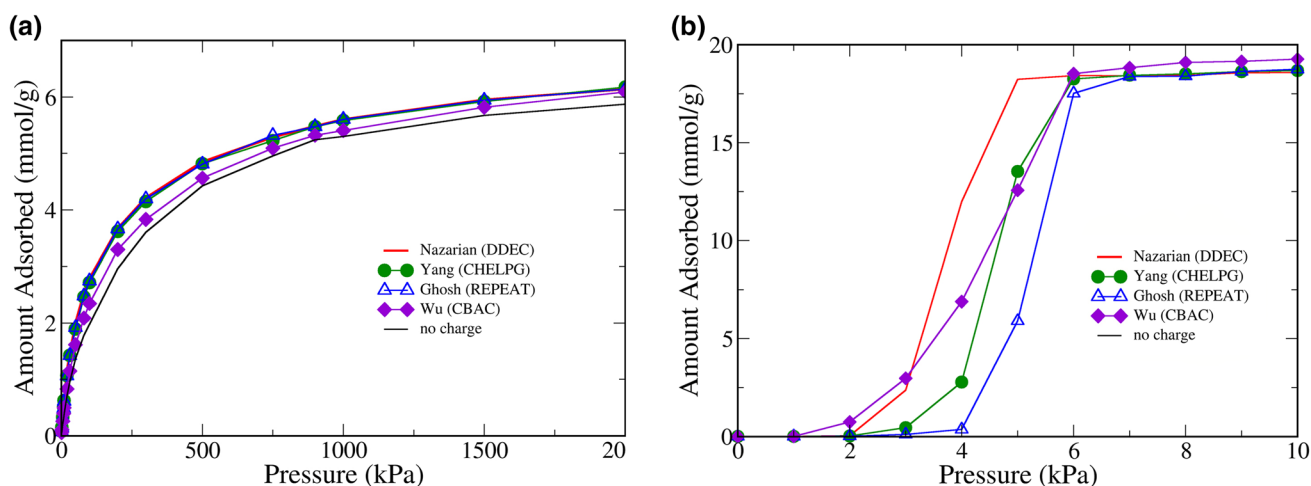


Fig. 9 Adsorption isotherms of: **a** CO₂; **b** water in UiO-66 at 298 K using different point charge sets for the framework atoms. Isotherms calculated without any framework charges are shown as a black line

(too low to be visible in the water plot). Error bars are the size of the symbols used

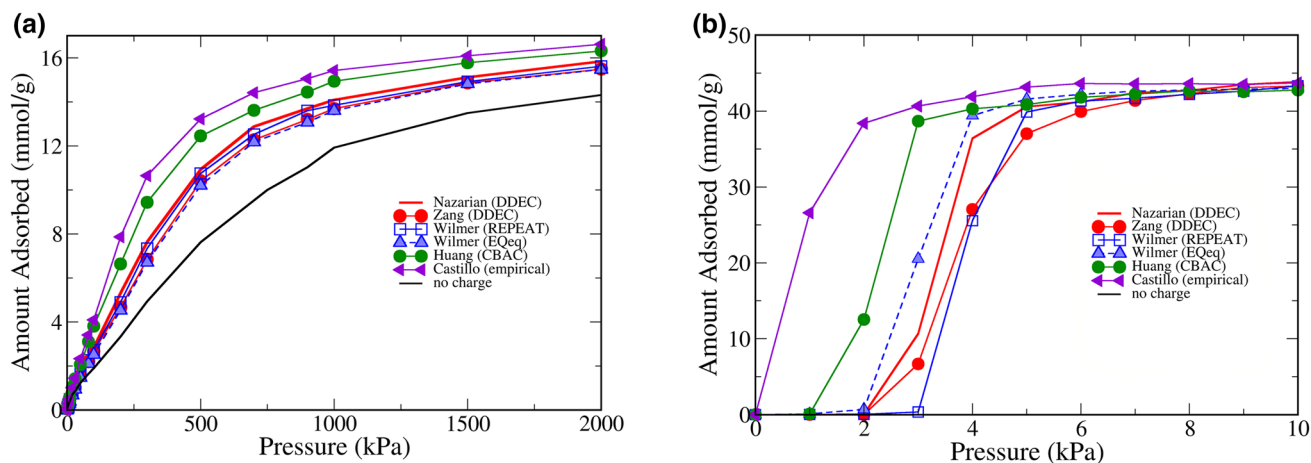


Fig. 12 Adsorption isotherms of: **a** CO₂; **b** water in CuBTC at 298 K using point charge sets obtained by periodic QM and semi-empirical methods. Isotherms calculated without any framework charges are

shown as a black line (too low to be visible in the water plot). Error bars are the size of the symbols used

the periodic sets of Nazarian, Wilmer and Zang have the smallest slopes and Cu charges around + 0.9. The correlation is not perfect, however, with the Yazaydin1 set showing a steep slope and relatively low Cu charge, while the Yazaydin2 set has a relatively smaller slope and a higher Cu charge.”

3.5 Co-MOF-74

In Table 5, the charge on the Co atom for the Wilmer and Snurr (2011) EQeq charge set should be 1.164 and not 0.164 as originally reported by mistake.

In the last paragraph of section 3.5, beginning in page 679 of the original paper [1], the sentences:

“Conversely, the EQeq method has by far the lowest charge on the metal, and consequently predicts the lowest adsorbed amount for water. However, the same is not observed in the CO₂ isotherm, for which the EQeq isotherm is the second largest. It is clear that the effect of electrostatic potential around the metal site has a much more pronounced effect on water adsorption, as observed above for CuBTC. Co-MOF-74 has a large number of OMS facing the hexagonal pores, which explains the high sensitivity of the adsorption prediction on the metal centre charge. Unlike the rest of the studied MOFs, the type V isotherm due to weak water-adsorbent interactions is not observed here. Again, this is likely to result from the high concentration

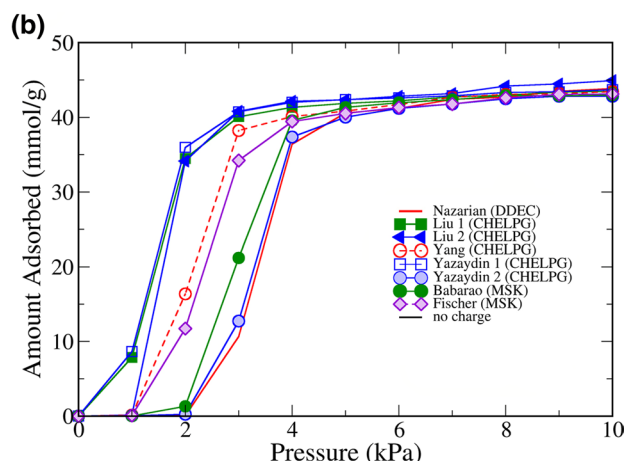
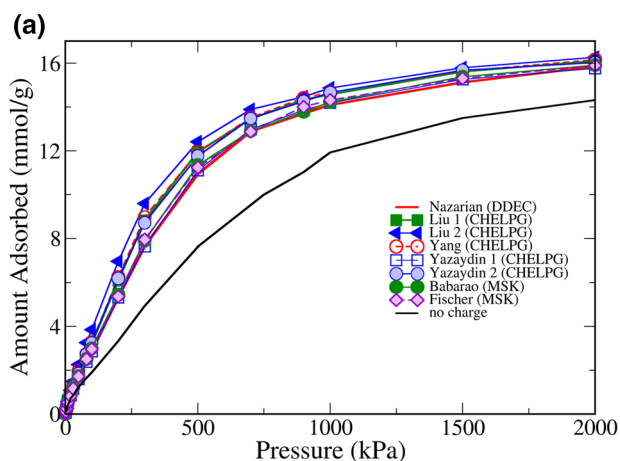


Fig. 13 Adsorption isotherms of: **a** CO₂; **b** water in CuBTC at 298 K comparing DDEC point charges to charges obtained by cluster methods. Isotherms calculated without any framework charges are shown

as a black line (too low to be visible in the water plot). Error bars are the size of the symbols used

of OMS pointed directly into the pore channel, facilitating the interaction between these sites and the water molecules. Finally, it is important to note that once again most of the QM-based charge sets, with the exception of LoProp as discussed above, lead to consistent isotherms for both gases.” should be replaced by:

“Conversely, the EQeq method has by far the lowest charge on the metal, but strangely this does not seem to significantly affect the uptake of both gases. This suggests that the charge magnitude on the metal site has a less pronounced effect on adsorption than observed above for CuBTC. Unlike

the rest of the studied MOFs, the type V isotherm due to weak water-adsorbent interactions is not observed here. This is likely to result from the high concentration of OMS pointed directly into the pore channel of Co-MOF-74, facilitating the interaction between these sites and the water molecules. Finally, it is important to note that once again most of the QM-based charge sets, perhaps with the exception of LoProp as discussed above, lead to consistent isotherms for both gases.”

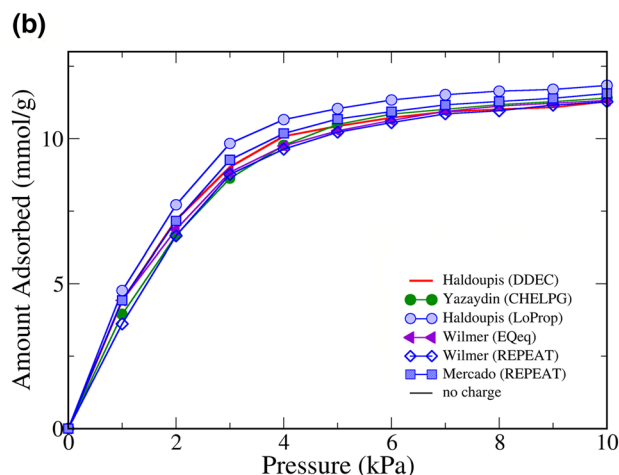
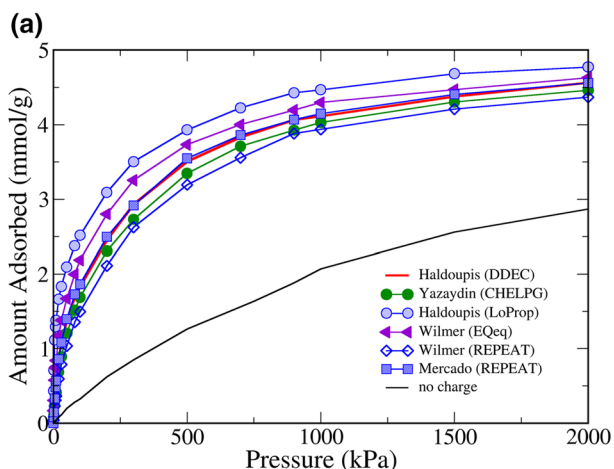


Fig. 15 Adsorption isotherms of: **a** CO₂; **b** water in Co-MOF-74 at 298 K using different point charge sets for the framework atoms. A plot of the water isotherms using a larger pressure range is provided

in Figure S14. Isotherms calculated without any framework charges are shown as a black line (too low to be visible in the water plot). Error bars are the size of the symbols used

References

1. Sladekova, K., Campbell, C., Grant, C., Fletcher, A., Gomes, J., Jorge, M.: The effect of atomic point charges on adsorption isotherms of CO₂ and water in metal organic frameworks. *Adsorption* **26**(5), 663–685 (2019)
2. Berendsen, H., Grigera, J., Straatsma, T.: The missing term in effective pair potentials. *J. Phys. Chem.* **91**, 6269–6271 (1987)

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