# Understanding $CO_2$ adsorption mechanisms in different diamine-appended metal-organic frameworks: A systematic DFT study combined with NMR chemical shift simulations

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Diamine-appended metal-organic frameworks (MOFs) have been considered as promising candidates for $CO_2$ capture due to their high working capacities and strong selectivity for $CO_2$ caused by a cooperative adsorption mechanism. Here we investigate $CO_2$ adsorption mechanisms in twelve different diamine-appended MOFs using van der Waals (vdW)-corrected density functional theory (DFT) combined with nuclear magnetic resonance (NMR) chemical shift simulations. Our vdW-corrected DFT calculations accurately predict $CO_2$ binding enthalpies and $^1$H, $^{13}$C, and $^{15}$N NMR chemical shifts. Based on this agreement, we find that eleven cases of twelve diamine-appended MOFs are likely to form ammonium carbamate geometries while for dmpn-appended MOF a mixed mechanism between the ammonium carbamate and the carbamic acid geometries is proposed.

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