Energy & Environmental Science

Electronic supplementary information

Exceptionally high CO_2 storage in covalent-organic frameworks: Atomistic simulation study

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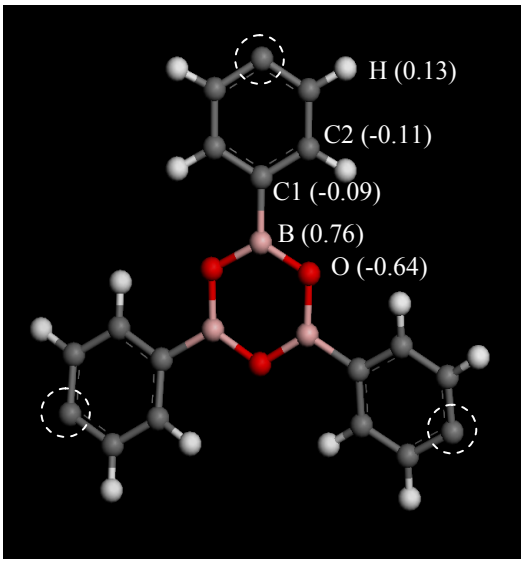
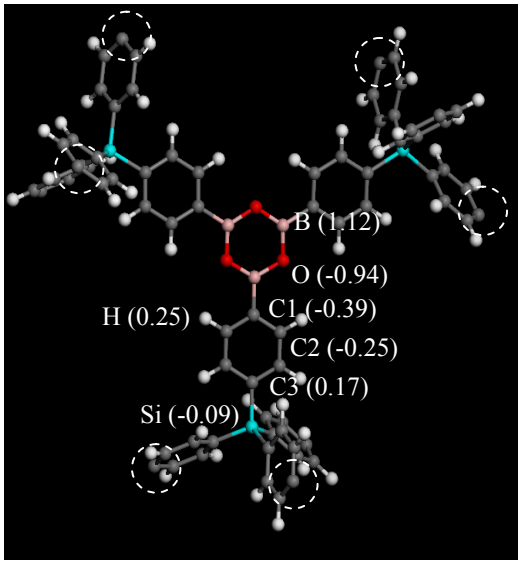
Figure S1. Atomic charges in COF-102, COF-103, COF-105, COF-108, COF-6, COF-8, COF-10 and COF_NT. Different cluster models were used in the density-functional theory calculations. The dangling bonds (indicated by dashed circles) in the cleaved clusters were terminated by methyl group to maintain the correct hybridization.

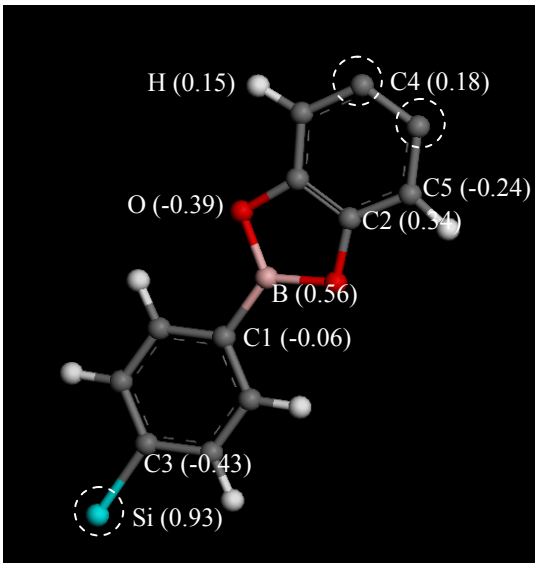
COF-102



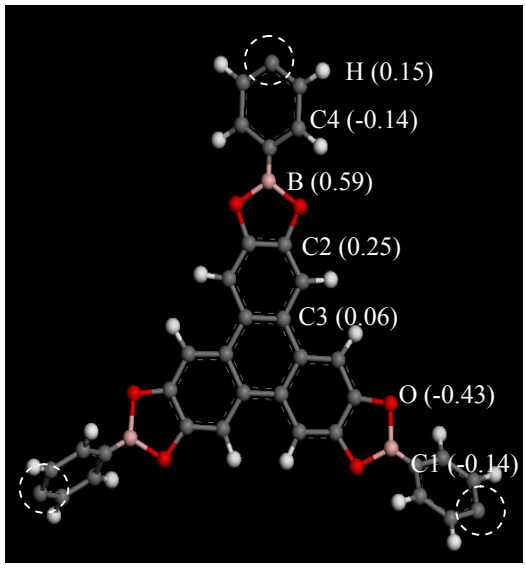
COF-103



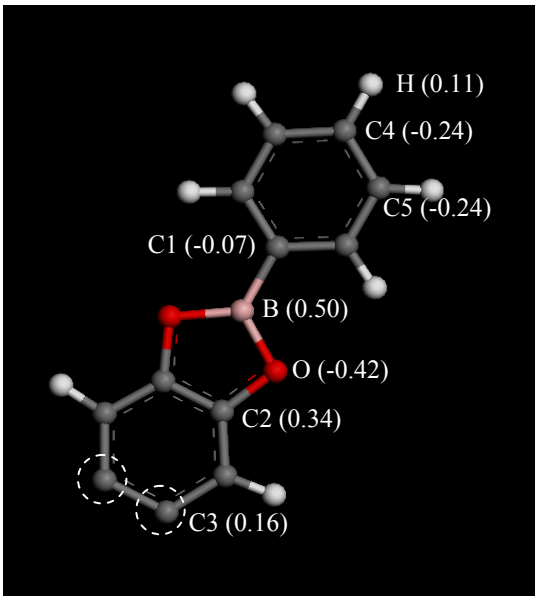
COF-105



COF-108



COF-6, COF-8 and COF-10



COF_NT