

Supporting Information for: CO₂ capture using boron, nitrogen, and phosphorus-doped C₂₀ in the present electric field: DFT study

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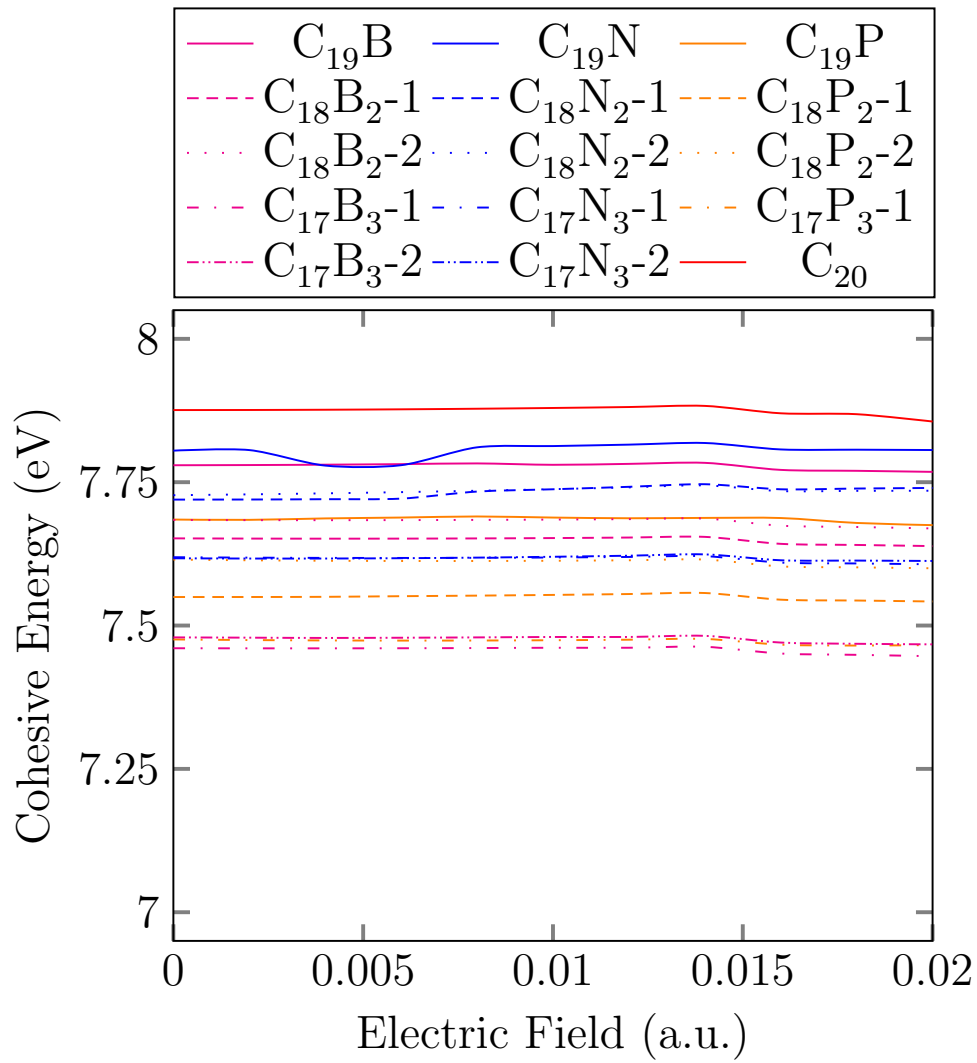


Figure S1: Variation of cohesive energy for C_{20} and $C_{20-n}X_n$ ($n= 1, 2$, and 3 ; $X= B, N$, and P) in $0-0.02$ *a.u.* electric field.

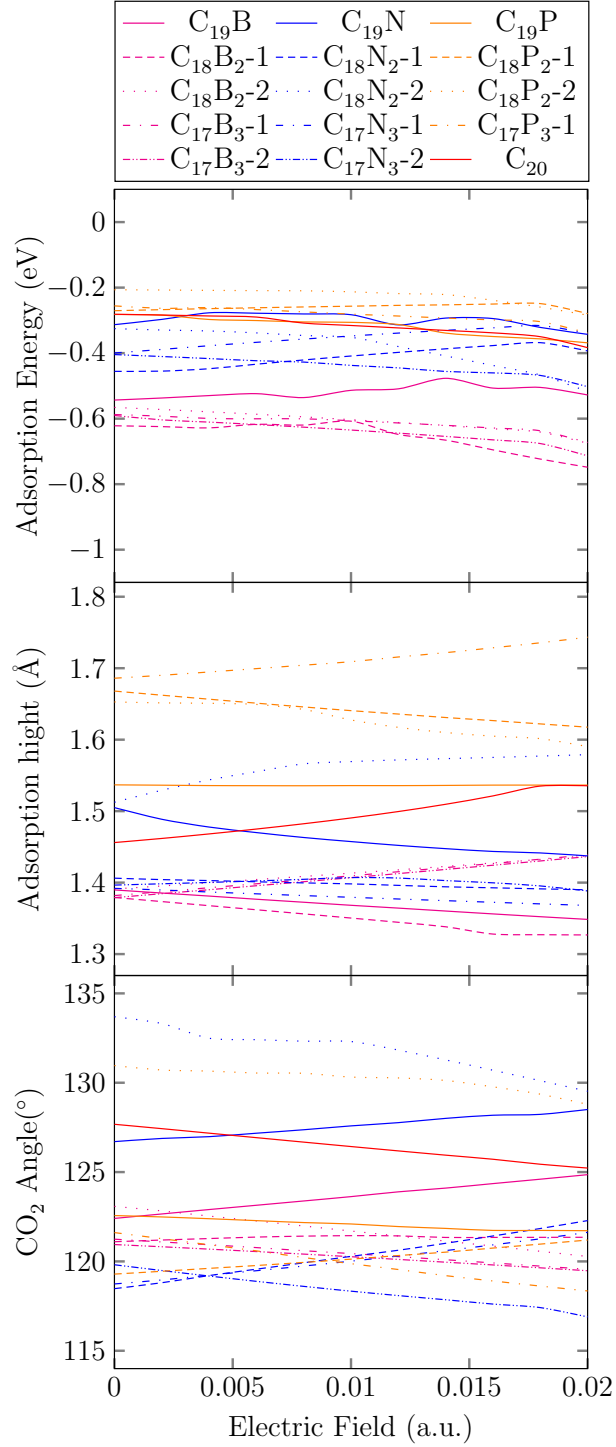


Figure S2: Variation of (a) adsorption energy (eV) (b) adsorption height (Å) (c) CO_2 angle (°) for C_{20} and $C_{20-n}X_n$ ($n=1, 2$, and 3 ; $X=B, N$, and P) in $0 - 0.02$ a.u. electric field.