

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

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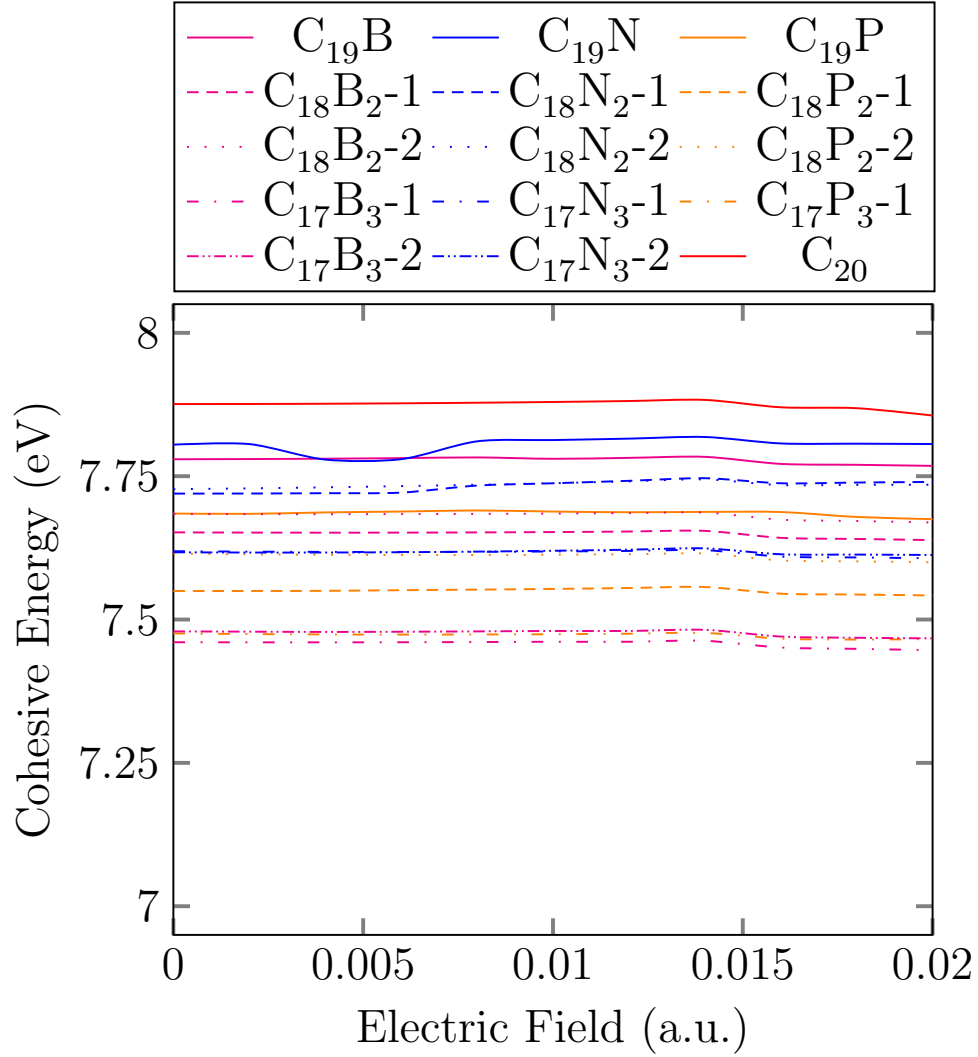


Figure S1: Variation of cohesive energy for C_{20} and $C_{20-n}X_n$ ($n=1, 2, \text{ and } 3$; $X= B, N, \text{ and } P$) in 0–0.02 *a.u.* electric field.

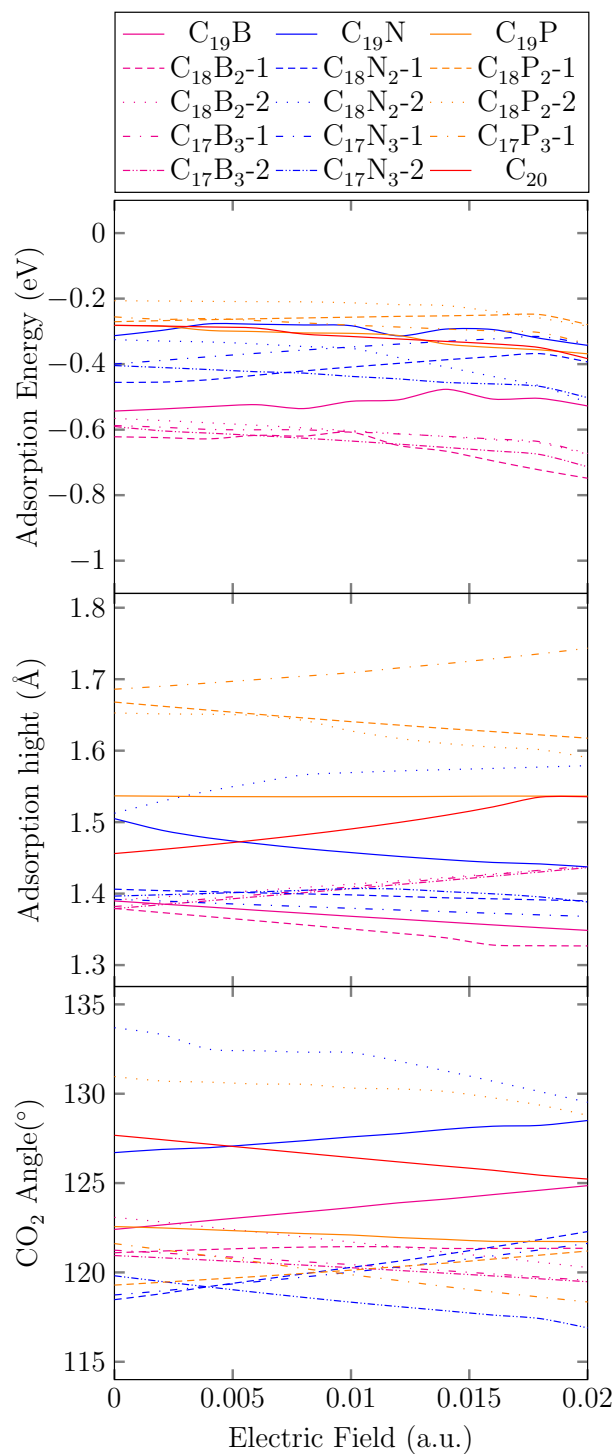


Figure S2: Variation of (a) adsorption energy (eV) (b) adsorption height (Å) (c) CO₂ angle (°) for C₂₀ and C_{20-n}X_n (n=1, 2, and 3; X=B, N, and P) in 0 – 0.02 *a.u.* electric field.