

“Supplementary Materials”

Reversible CO₂ storage and efficient separation using Ca decorated porphyrin-like porous C₂₄N₂₄ fullerene: A DFT study

Mehdi D. Esrafilⁱ *^a and Sharieh Hosseini^b

^a Department of Chemistry, Faculty of Basic Sciences, University of Maragheh, P.O. Box 55136-553, Maragheh, Iran

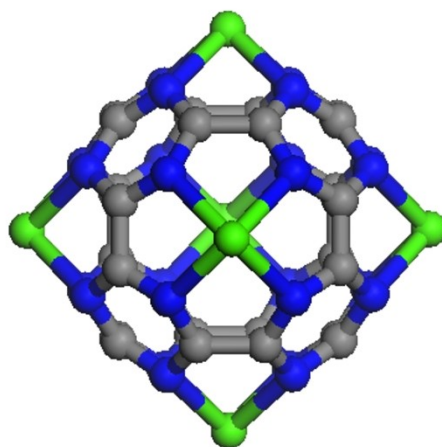
^b Department of Chemistry, Faculty of Pharmaceutical Chemistry, Tehran Medical Sciences, Islamic Azad University, Tehran, Iran

Phone: (+98) 4212237955. **Fax:** (+98) 4212276060. **P.O. Box:** 5513864596. **E-mail:** esrafilⁱ@maragheh.ac.ir

* Corresponding author. **E-mail:** esrafilⁱ@maragheh.ac.ir (M. D. Esrafilⁱ).

Figure S1. (a) The geometries of $\text{Ca}_6\text{C}_{24}\text{N}_{24}$ after the MD simulations (2000 fs, at 600 K) and (b) the variation of potential energy of this system with the time

(a)



(b)

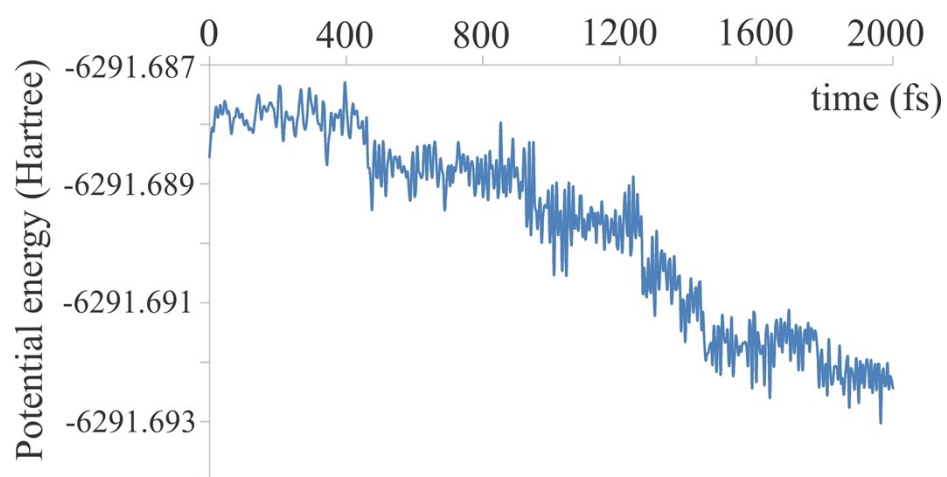


Figure S2. Molecular graphs of CO₂ adsorbed structures on CaC₂₄N₂₄: (a) 1CO₂@CaC₂₄N₂₄, (b) 2CO₂@CaC₂₄N₂₄, (c) 3CO₂@CaC₂₄N₂₄, (d) 4CO₂@CaC₂₄N₂₄, (e) 5CO₂@CaC₂₄N₂₄ and (f) 24CO₂@CaC₂₄N₂₄. The small red circles indicate the BCPs.

