

“Supplementary Material”

Alkali metal decorated C₆₀ fullerenes as promising materials for delivery of anticancer 5-fluorouracil drug: A DFT approach

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Figure S1. The energy profile for the migration of the Li atom from above the hexagon ring to neighboring pentagon ring. The IS, TS and FS shows the initial state, transition state and final state, respectively.

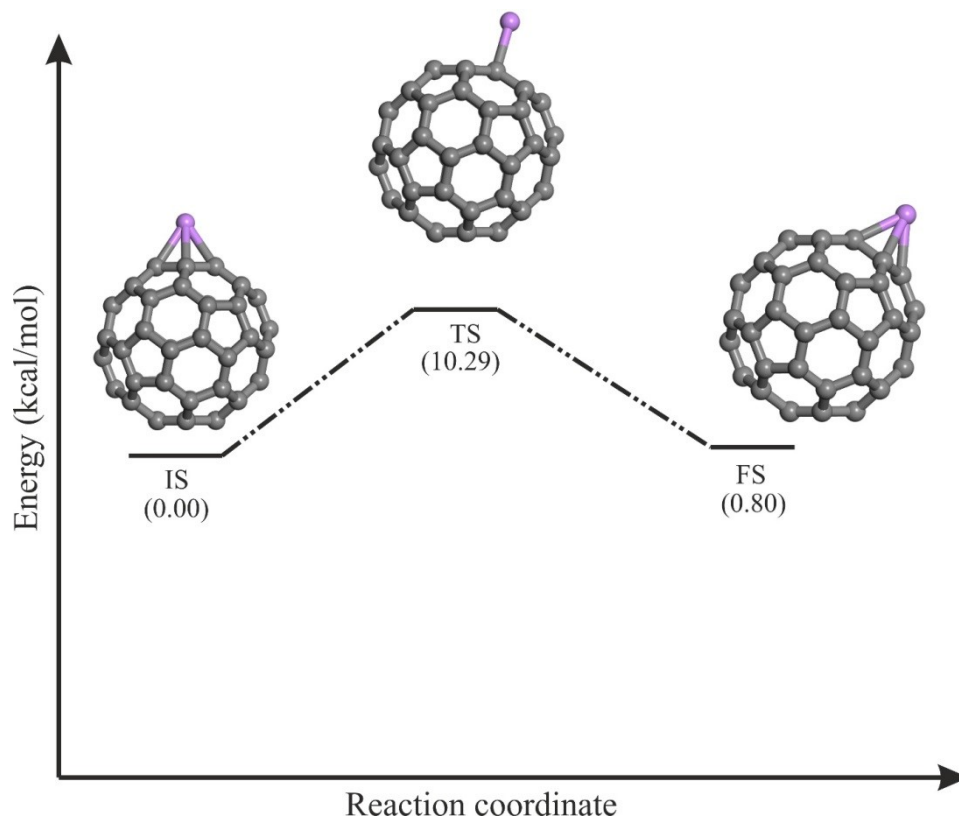
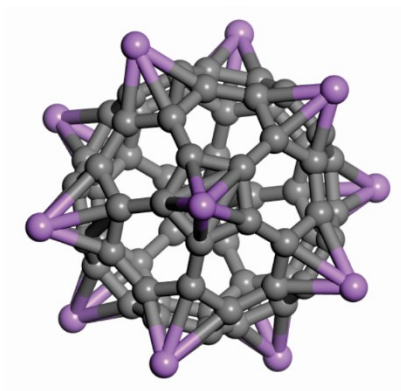
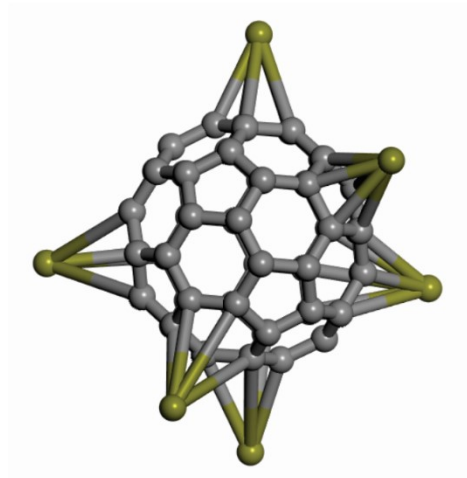


Figure S2. The final structure of (a) $\text{Li}_{12}/\text{C}_{60}$, (b) $\text{Na}_6/\text{C}_{60}$ and (c) K_6/C_{60} after the MD simulations at 300 K and for 5000 fs

(a)



(b)



(c)

