nanomaterials

Supplementary Material

Interaction in Li@Fullerenes and Li+@fullerenes: First Principle Insights to Li-based Endohedral Fullerenes

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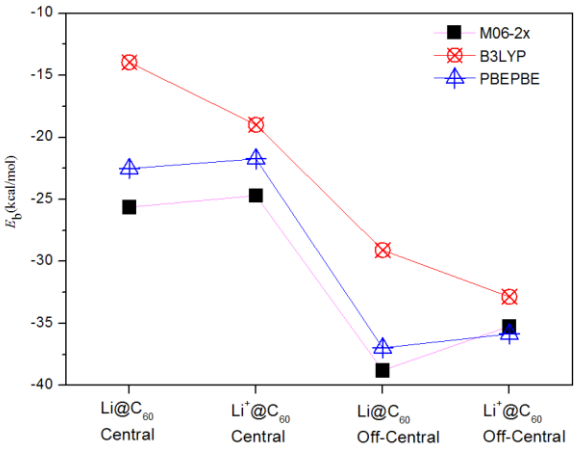

Figure S1. The binding energy of $Li@C_{60}$ and $Li^{+}@C_{60}$ obtained by PBEPBE, B3LYP and M06-2X methods

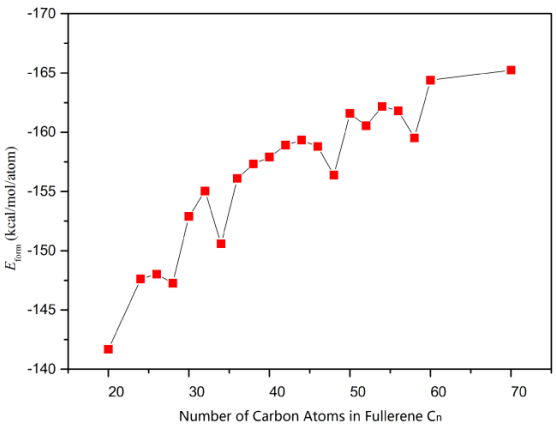

Figure S2. The formation energy of the empty cages (in kcal/mol/atom)