# Supporting Information

## Reducing the Polyaromatic Hydrocarbons: the Capability and Capacity of Lithium

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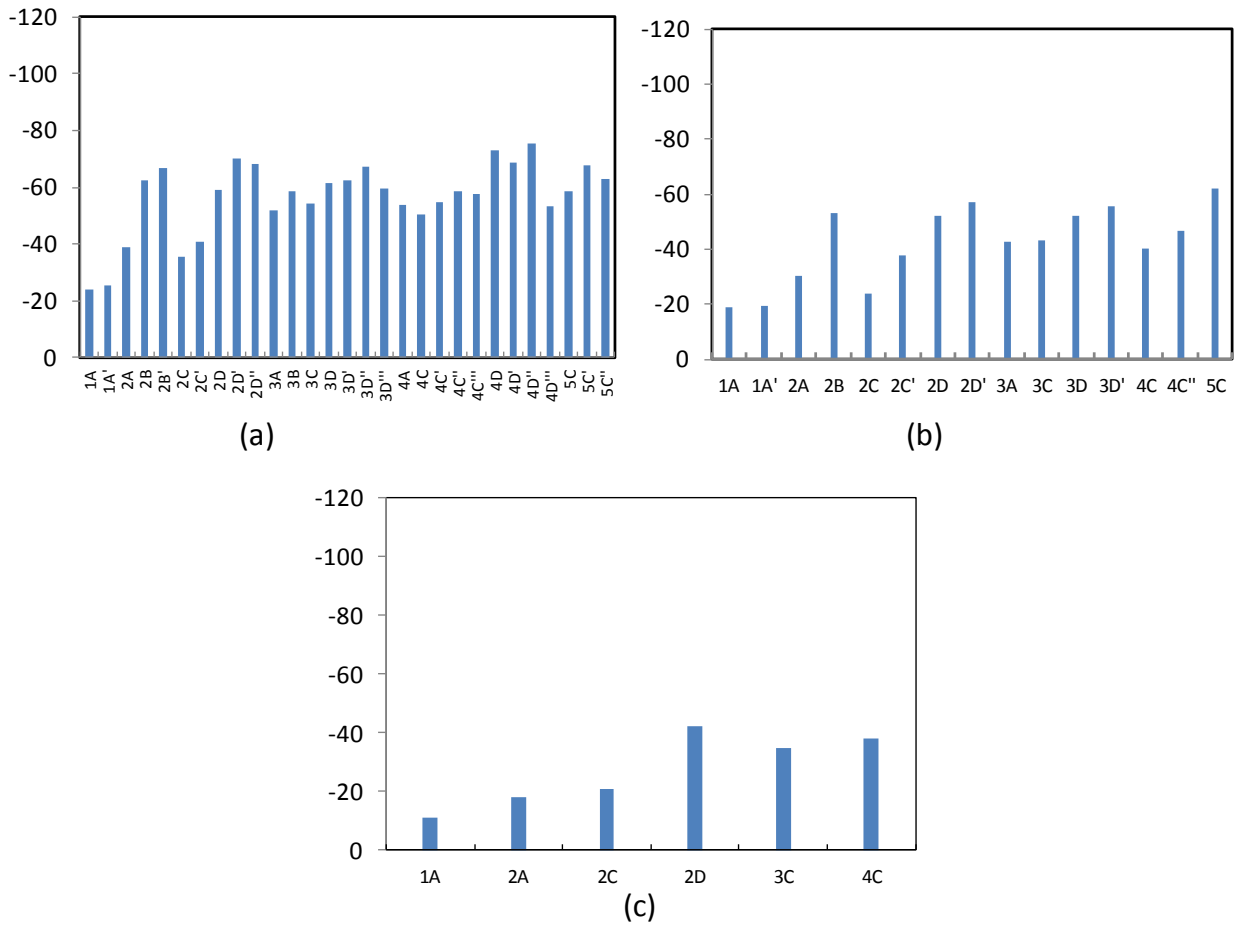
Supporting table I. Binding energy (in kcal/mol) calculated by different quantum chemical levels for the PAH-Li complex systems..

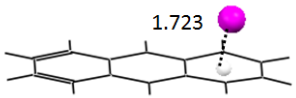
| Method | B-1A | B-2C | N-1A | N-2A | N-2C | N-2D | N-3C | N-4C |
|---|---|---|---|---|---|---|---|---|
| [a]**MP2/6-31G(d)** | -7.60 | -48.90 | -13.10 | -22.39 | -64.11 | -72.47 | -31.44 | -65.02 |
| [a]**B3LYP/cc-pVTZ** | -1.84 | -48.03 | -23.13 | -42.54 | -63.93 | -73.67 | -65.61 | -42.71 |
| [a]**M062X/cc-pVTZ** | -5.78 | -58.07 | -30.65 | -54.69 | -77.33 | -88.74 | -48.98 | -59.16 |
| [a]**B3LYP/6-311++G(d)** | -1.68 | -47.61 | -23.00 | -42.15 | -63.58 | -73.11 | -64.88 | -41.73 |
| [a]**B3LYP/aug-cc-pVDZ** | -1.30 | -46.32 | -22.19 | -40.73 | -62.29 | -71.61 | -63.31 | -39.83 |
| [a]**B3PW91/6-31G(d)** | -3.48 | -47.20 | -21.73 | -44.37 | -63.77 | -74.23 | -67.70 | -44.77 |
| [a]**MP2/cc-pVTZ** | -4.75 | -56.30 | -19.83 | -52.77 | -73.37 | -97.06 | -45.62 | -71.14 |
| [a]**ωB97XD/6-31G(d)** | -5.64 | -49.95 | -23.40 | -41.92 | -68.52 | -80.57 | -73.97 | -43.71 |
| [a]**B2PLYP/6-311++G(d)** | -3.27 | -49.08 | -21.94 | -44.25 | -65.06 | -74.16 | -68.64 | -52.14 |
| [b]**B3LYP/6-31G(d)** | -5.78 | -49.19 | -18.47 | -41.44 | -57.40 | -69.14 | -62.32 | -54.81 |

[a] Energy calculated on the MP2/6-31G(d) geometries

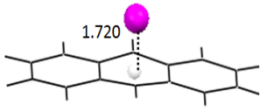
[b] Energy calculated on the B3LYP/6-31G(d) geometries



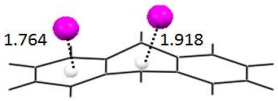

Supporting figure I. The total interaction energy (IE2) in kcal/mol of the B3LYP/6-31G(d) (a) T-Li (b) A-Li (c) N -Li complexes. The B.E and D.E are in kcal/mol, while the natural charges are in a.u.



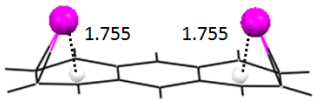

**A-1A** (-22.57)



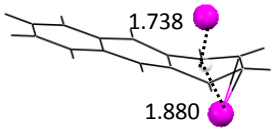

**A-1A'** (-24.20)



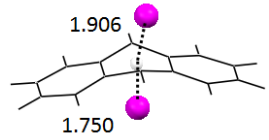

**A-2A** (-56.02)



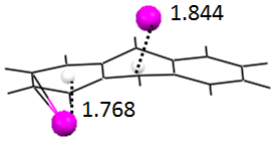

**A-2B** (-65.41)



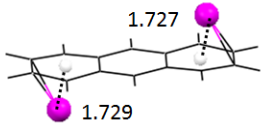

**A-2C** (-58.52)



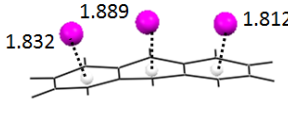

**A-2C'** (-66.11)



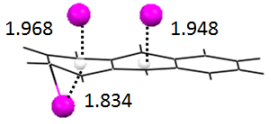

**A-2D** (-76.38)



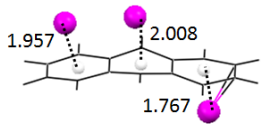

**A-2D'** (-66.86)



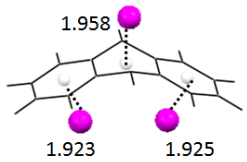

**A-3A** (-53.83)



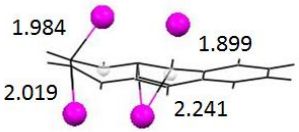

**A-3C** (-62.32)



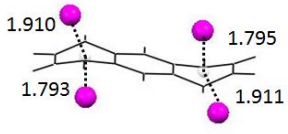

**A-3D** (-69.86)



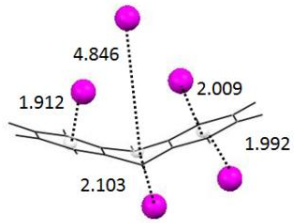

**A-3D'** (-99.93)



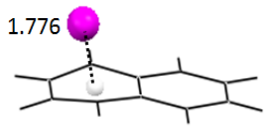

**A-4C** (-85.09)



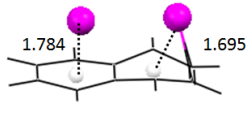

**A-4C''** (-98.26)



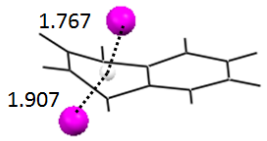

**A-5C** (-92.57)



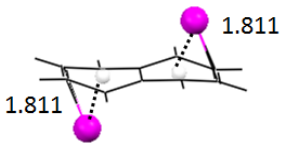

**N-1A** (-18.47)



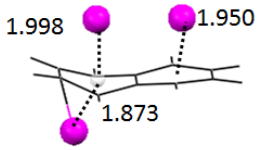

**N-2A** (-41.44)



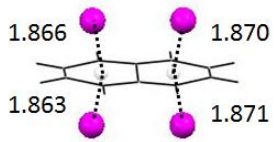

**N-2C** (-57.40)



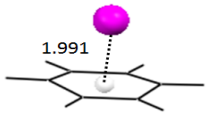

**N-2D** (-69.14)



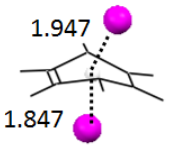

**N- 3C** (-62.32)




**N-4C** (-54.81)




**B-1A** (-5.78)




**B-2C** (-49.19)

Supporting figure II. All possible B3LYP/6-31G(d) optimized geometry of the mono, di, tri, tetra and penta lithium anthracene, naphthalene, and benzene complexes. Binding energy values are given in kcal/mol and the Li... ring centroid distances are given in Å.