

Doped Hexa-*peri*-hexabenzocoronene as Anode Material in Lithium- and Magnesium-Ion Batteries

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Table S1. Comparison of our results for adsorption energies with literature values.

Adsorption energies in kcal/mol.

system	literature	our study	% difference
Li ⁺ /C ₃₆ H ₁₈ B ₃ N ₃	-47.9	-50.81	-6.08
Li/C ₃₆ H ₁₈ B ₃ N ₃	-25.2	-16.40	34.92
Li ⁺ /C ₄₂ H ₁₈	-53.3	-51.57	3.25
Li/C ₄₂ H ₁₈	-13.8	-17.39	-26.01
Mg/C ₄₂ H ₁₈	-4.10	-3.17	22.68
Mg ²⁺ /C ₄₂ H ₁₈	-189.2	-178.09	5.87

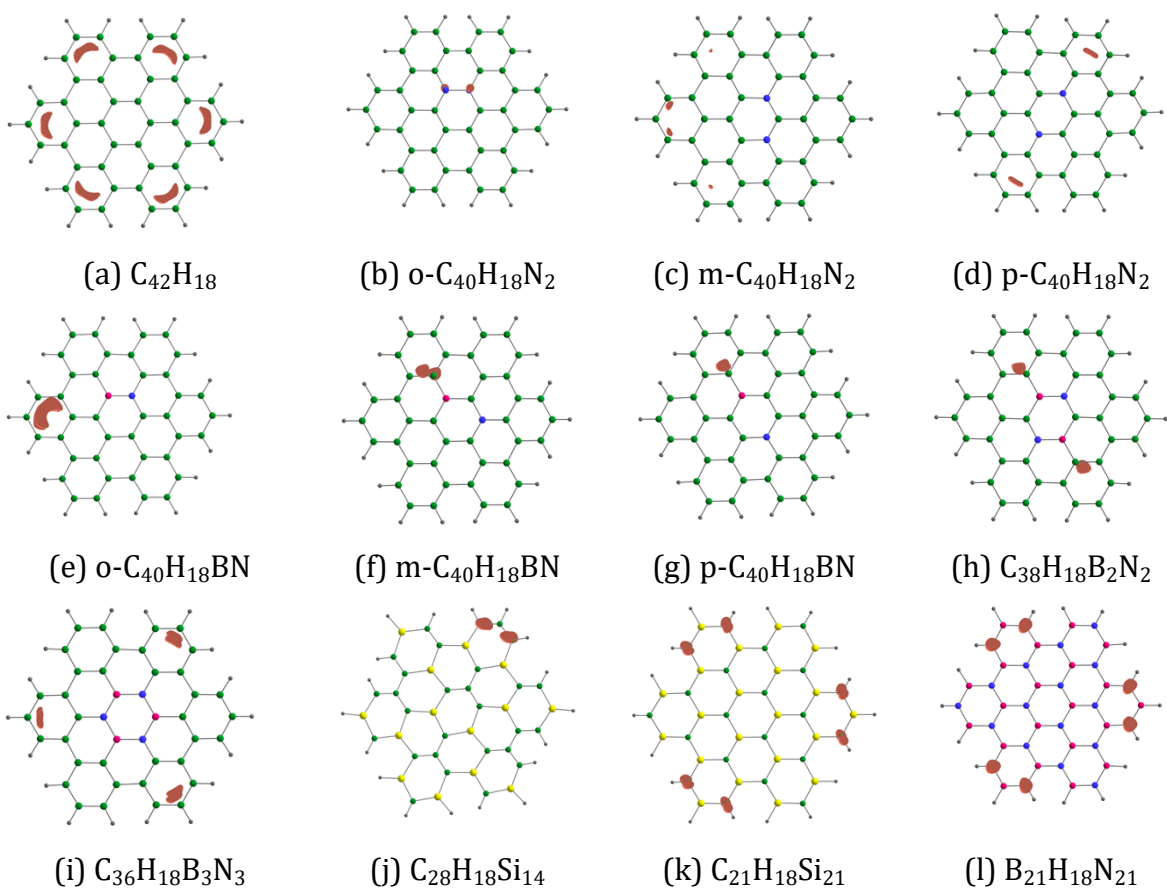


Figure S1. MESP V_{\min} features of (a) $C_{42}H_{18}$, (b) $o-C_{40}H_{18}N_2$, (c) $m-C_{40}H_{18}N_2$ (d) $p-C_{40}H_{18}N_2$, (e) $o-C_{40}H_{18}BN$, (f) $m-C_{40}H_{18}BN$, (g) $p-C_{40}H_{18}BN$, (h) $C_{38}H_{18}B_2N_2$, (i) $C_{36}H_{18}B_3N_3$, (j) $C_{28}H_{18}Si_{14}$, (k) $C_{21}H_{18}Si_{21}$, (l) $B_{21}H_{18}N_{21}$.

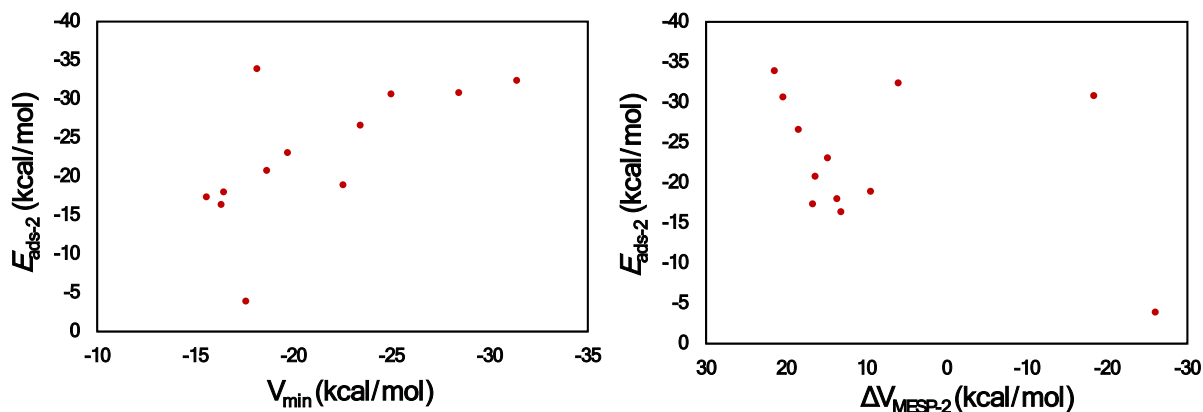


Figure S2. Correlation between (a) V_{\min} and $E_{\text{ads-2}}$ and (b) $\Delta V_{\text{MESP-2}}$ and $E_{\text{ads-2}}$ for Li-adsorbed HBCs.

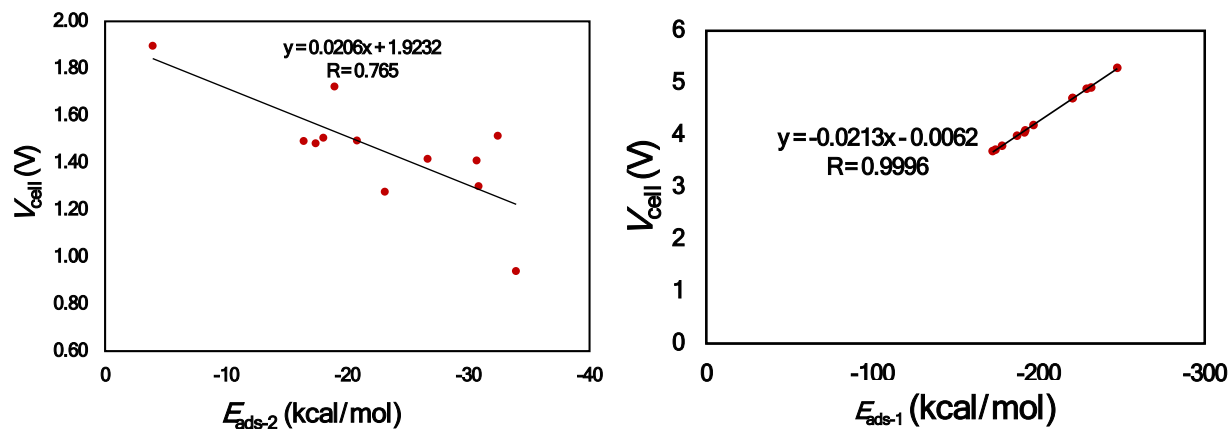


Figure S3. Correlation between (a) $E_{\text{ads-2}}$ and V_{cell} for doped HBCs for LIBs and (b) $E_{\text{ads-1}}$ and V_{cell} for doped HBCs for MIBs

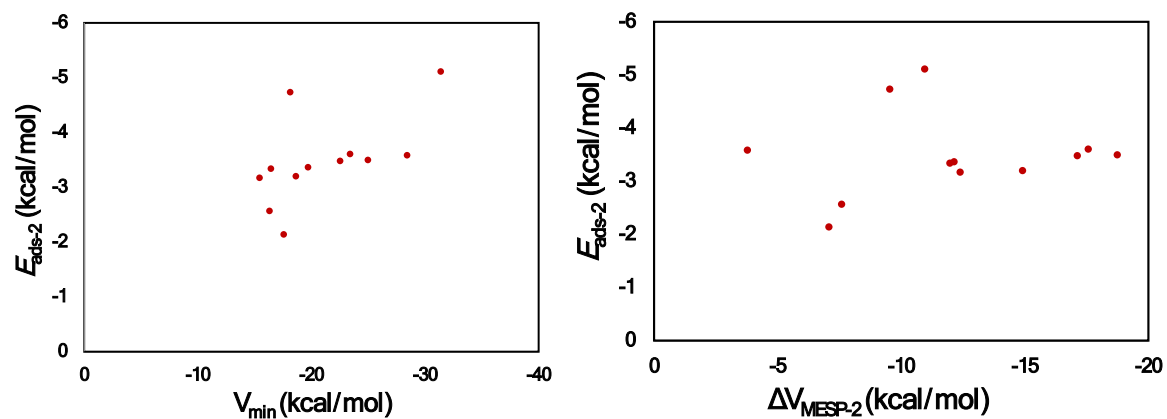


Figure S4. Correlation between (a) V_{min} and $E_{\text{ads-2}}$ and (b) $\Delta V_{\text{MESP-2}}$ and $E_{\text{ads-2}}$ for Mg-adsorbed HBCs.