Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information for

High-Performance Lithium/Sulfur Batteries by Decorating CMK-3/S with Fine-amount DNA

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Computational Details:

The first-principles calculations were conducted using density functional theory (DFT) method under generalized gradient approximations (GGA) framework where the Perdew-Wang (PW91[1]) functional was employed to describe the exchange-correlation. A double numerical basis set augmented with polarization functions was used to describe the valence electrons, while the core electrons were described by effective core pseudopotential method. The chosen computational scheme enables high quality results with only very little superposition effects. Due to the open-shell nature of the deoxyribonucleotides and the polysulfides, we used the spin-polarized scheme throughout the calculations to fully relax the structures without symmetry constraints using the conjugated gradient algorithm.[2-4] The molecular interaction energy E_{ads} was calculated by $E_{ads} = E_D + E_{Li_2S_8} - E_{D+Li_2S_8}$, where $E_{D+Li_2S_8}$, E_D and $E_{Li_2S_8}$ represent the energies of the Li_2S_8 adsorbed deoxyribonucleotides, the deoxyribonucleotides molecule and Li_2S_8, respectively. All calculations were carried out in the MS DMol[3] program.

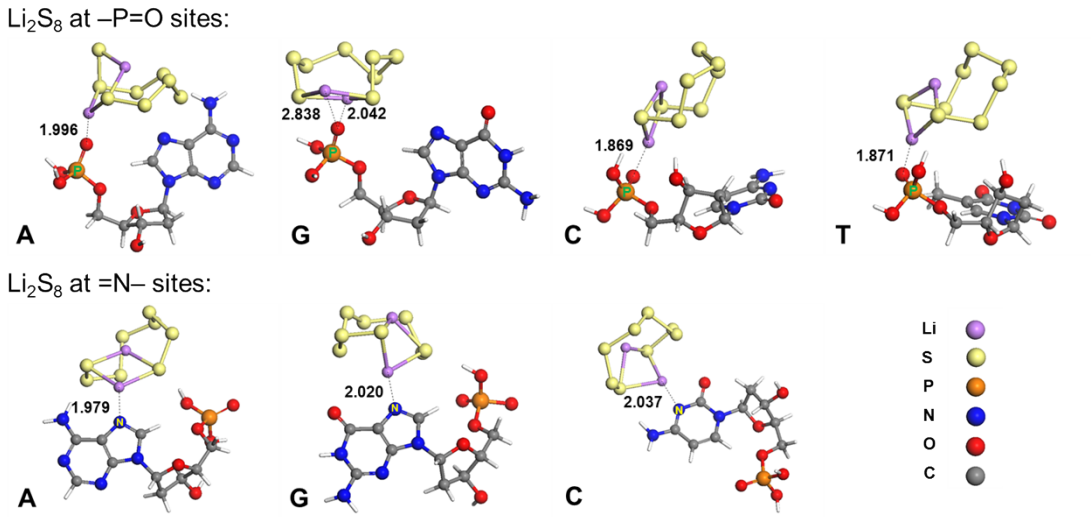

Figure S1. The most preferential adsorption structures of Li_2S_8 on the different groups of G deoxyribonucleotides. For G has all of the adsorption sites, we chose G to represent the adsorbed behaviours of Li_2S_8.

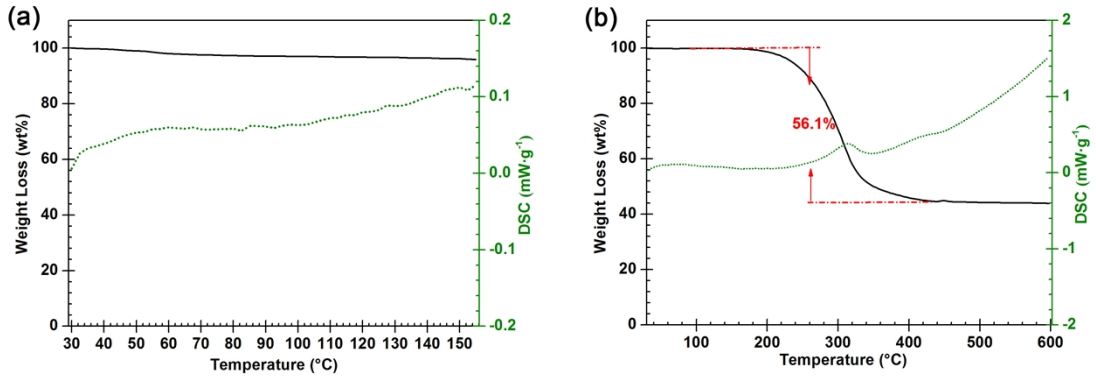

Figure S2. TGA (black solid line) and DSC (green dot line) curves. (a). Raw DNA powder; (b). CMK-3/S.

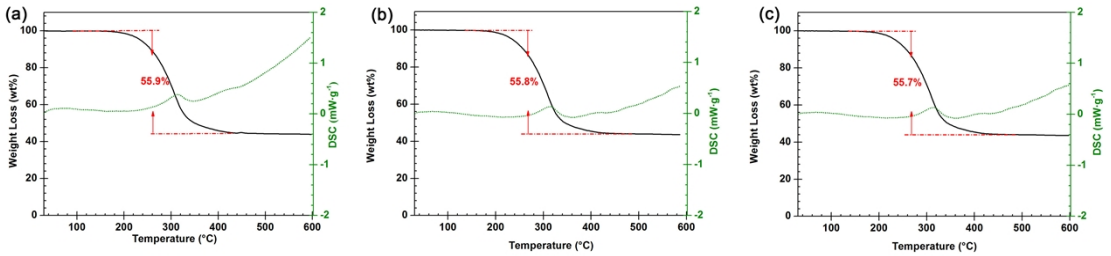

Figure S3. TGA (black solid line) and DSC (green dot line) curves. (a). CMK-3/D[**7**]/S; (b). CMK-3/D[**14**]/S; (c). CMK-3/D[**22**]/S.

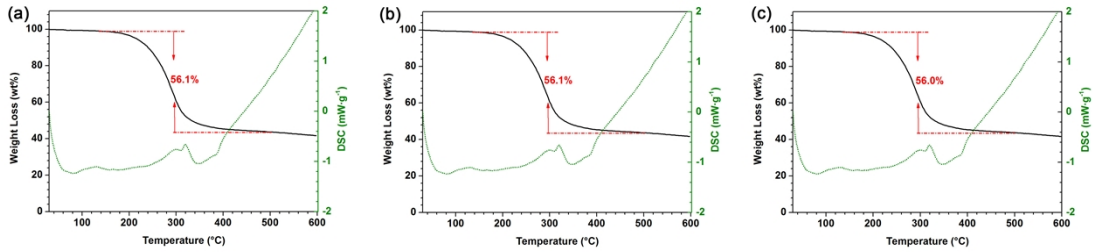

Figure S4. TGA (black solid line) and DSC (green dot line) curves. (a). CMK-3/S/D[**7**]; (b). CMK-3/S/D[**14**]; (c). CMK-3/S/D[**22**].

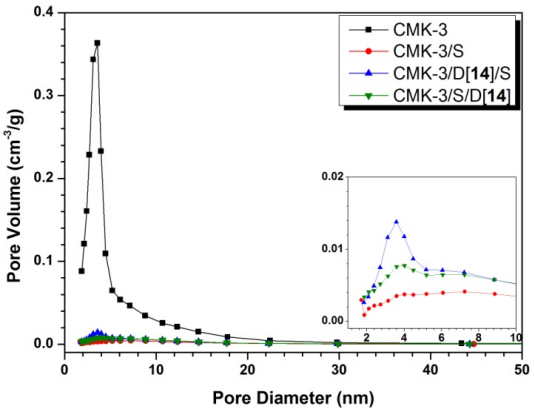

Figure S5. BJH mesopore distributions of CMK-3, CMK-3/S, CMK-3/D/S[14] and CMK-3/S/D[14].

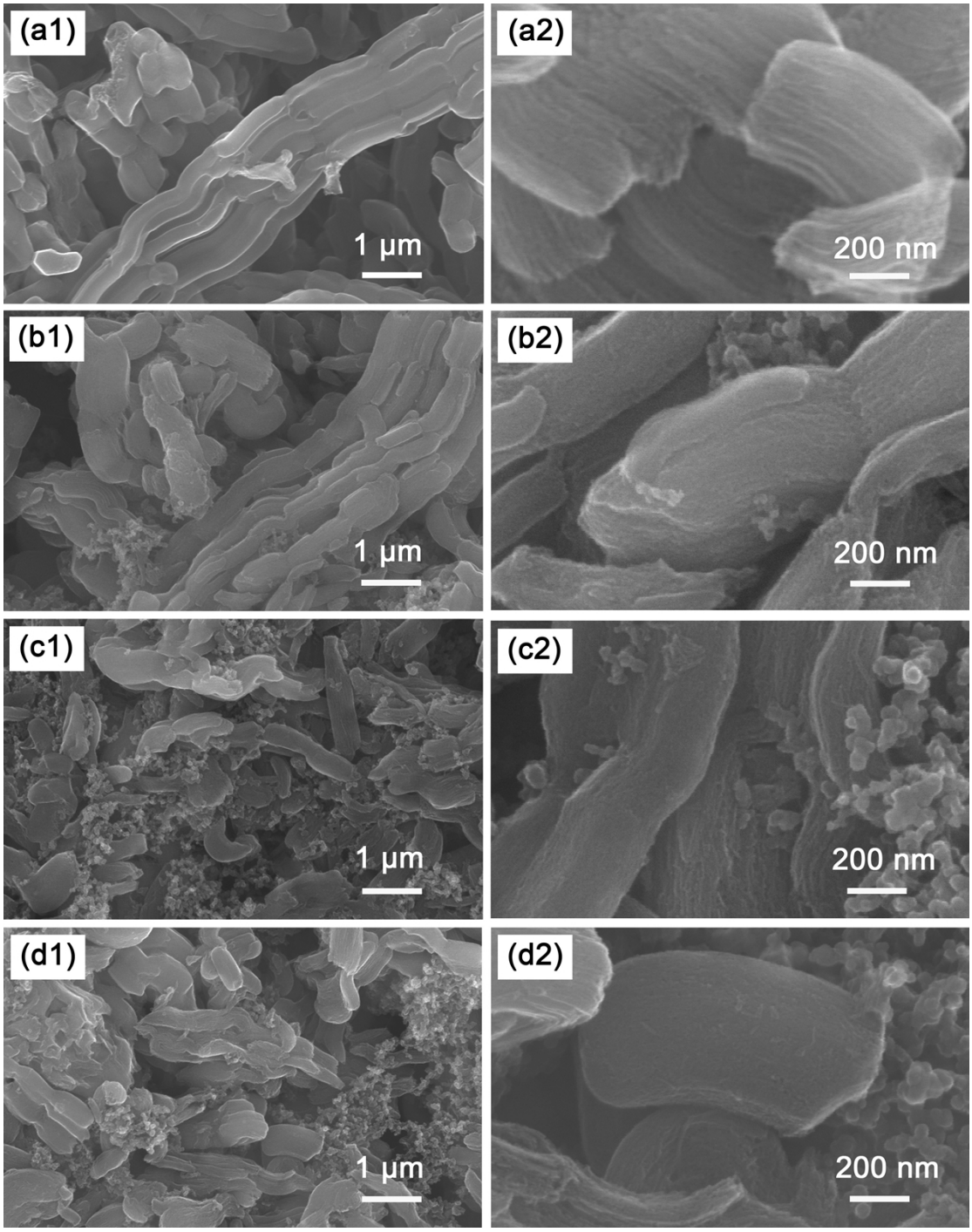

Figure S6. SEM images of bare CMK-3 (a1, a2), CMK-3/S (b1, b2), CMK-3/D[**14**]/S (c1, c2) and CMK-3/S/D[**14**] (d1, d2).

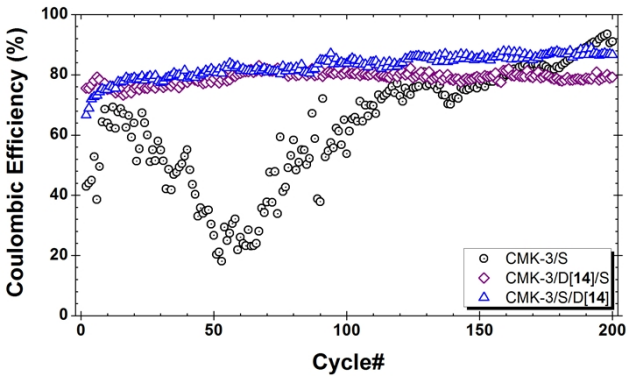

Figure S7. Coulombic efficiency of CMK-3/S, CMK-3/D[14]/S and CMK-3/S/D[14].

Table S1. Summary of sulfur weight ratio of TGA results.

Comp.	CMK-3/S	CMK-3/D[7]/S	CMK-3/D[14]/S	CMK-3/D[22]/S	CMK-3/S/D[7]	CMK-3/S/D[14]	CMK-3/S/D[22]
S (wt%)	56.1	55.9	55.8	55.7	56.1	56.1	56.0

Table S2. Summary of the specific surface area, pore volume and pore size measured through N_2 adsorption/desorption.

Sample	BET specific surface area($m^2 \cdot g^{-1}$)	Pore volume ($cm^3 \cdot g^{-1}$)	pore size (nm)
CMK-3	1117	1.37	3.6
CMK-3/S	38	0.08	8.8
CMK-3/D[**14**]/S	63	0.12	3.6
CMK-3/S/D[**14**]	54	0.11	4.0

Table S3. Fitted values for the equivalent circuit elements in Scheme **1** by simulation of EIS data in Figure 4.

Sample #	R_{el} (Ω)	C_{sl}($F \cdot cm^{-2}$)	R_{sl} (Ω)	CPE_1		R_{er} (Ω)	CPE_2	
				Y_1 ($\Omega^{-1} \cdot s^n$)	n_1		Y_2 ($\Omega^{-1} \cdot s^n$)	n_2
Before 1st Cycle								
CMK-3/S	1.357	4.112×10^{-6}	5.529	1.174×10^{-5}	0.813	53.58	0.070	0.805
CMK-3/D[**14**]/S	2.838	7.519×10^{-6}	7.812	3.492×10^{-5}	0.720	31.32	0.061	0.641
CMK-3/S/D[**14**]	6.449	1.112×10^{-5}	3.011	1.345×10^{-5}	0.787	73.40	0.094	0.774
After 200th cycles								
CMK-3/S	26.30	3.491×10^{-6}	10.86	1.876×10^{-2}	0.325	11.10	0.167	0.631
CMK-3/D[**14**]/S	2.062	4.291×10^{-6}	6.719	2.273×10^{-2}	0.234	23.38	0.053	0.823
CMK-3/S/D[**14**]	6.279	4.109×10^{-6}	5.489	1.202×10^{-4}	0.630	13.69	0.150	0.406

References:

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