Supporting information

High-capacity organic sodium ion batteries using sustainable C4Q/CMK-3/SWCNTs electrode

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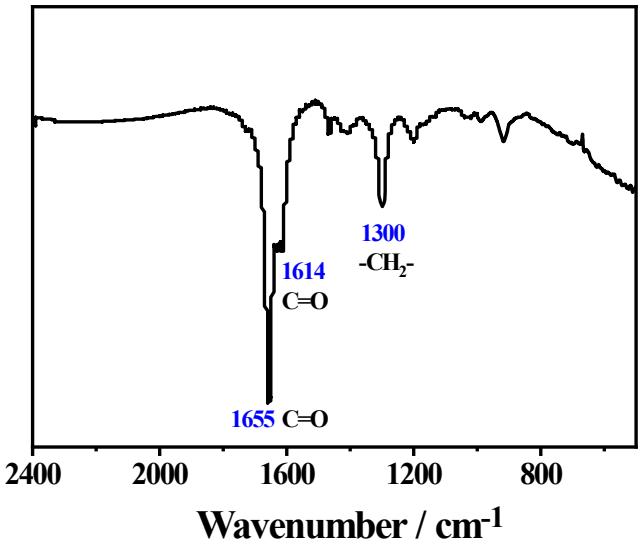

Figure S1 Infrared spectrum of C4Q

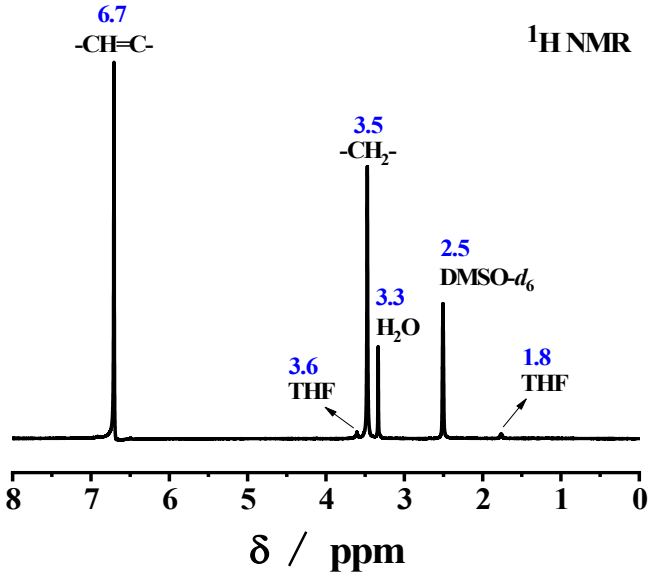

Figure S2 ^{1}H NMR spectrum of C4Q

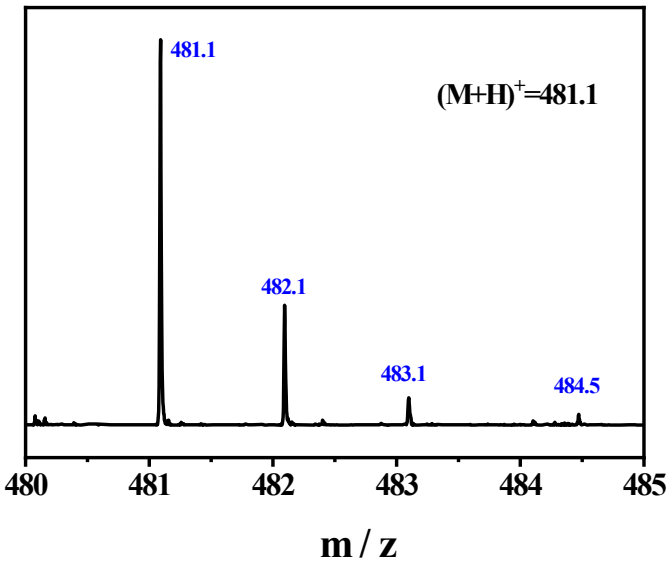

Figure S3 ESI-MS spectrum of C4Q

Computational Details

Density functional theory calculations were carried out using Gaussian 09W software package.[1] The geometries were fully optimized for each molecule using Becky's three-parameter exchange function combined with Lee-Yang-Parr correlation functional (B3LYP). [2] We initially optimized these structures at B3LYP/3-21G theoretical level and followed by a reasonable size of the basis set (6-31G*). Vibration spectra calculations were implemented to verify the true energy minima and to derive corrections for zero point energy. The average potential platform was speculated by calculating the standard Gibbs free energy of reaction.[3]

It is noted that most organic compounds that bear more than two carbonyl groups cannot reach their theoretical capacity because only half (if not less) of the carbonyl sites take part in reversible reactions with alkaline metal.[4] Our previous study has shown that the highest occupied molecular orbitals (HOMO) plotting is a practical and useful tool for the predication of carbonyl utilization. [5, 6] The computational details are described in the supporting information (Tables S1). Besides, the average potential platform for C4Q with sodium ion are predicted by calculating the standard Gibbs free energy of reaction,[7] as summarized in Table S2. The redox potential (E) of C4Q/Na_8C4Q is 2.228 V on the base of the equation $\Delta G=-ZFE$, where Z is the number of electron transfer, and F is the Faraday constant. This value is basically consistent with the actual discharge voltage.

Table S1. Cartesian Coordinates (Å) of the optimized structure for C4Q reduced with 8Na (C_1 symmetry) calculated at the RB3LYP/6-31G(d) Level.

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.21821	-1.035599	-1.121239	H	3.205313	-3.095691	-1.713118
C	-5.042604	-0.234408	0.351136	H	2.260167	-2.083258	-2.785267
C	-3.236795	1.283284	-0.373636	C	-2.513306	-2.239027	-1.734484
C	-2.638303	0.269890	-1.180601	H	-3.203946	-3.094241	-1.718379
C	3.218830	-1.036705	-1.118561	H	-2.257084	-2.080298	-2.787667
C	4.390538	-1.248866	-0.385229	C	-4.389059	-1.248969	-0.386807
C	5.044014	-0.233543	0.351704	H	-4.818448	-2.251215	-0.358220
C	4.412207	1.029665	0.345979	C	-4.411507	1.029220	0.345438
C	3.236708	1.282528	-0.372259	H	-4.853399	1.821562	0.949971
C	2.637951	0.268373	-1.177590	C	-1.21998	2.43212	0.62104
C	-1.20013	1.5998	1.748821	C	1.219811	2.432252	0.622083
C	0.000244	2.95489	0.109584	C	2.526236	2.612855	-0.158405
C	1.199307	1.599625	1.749699	H	2.287737	3.106016	-1.107872
C	-0.000369	1.164602	2.372826	H	3.209765	3.288616	0.377700

C	-1.215961	-2.580207	-1.003390	O	6.149847	-0.465416	1.044194
C	-1.196654	-2.670090	0.398646	O	1.509626	0.508145	-1.878408
C	-0.000781	-2.766557	1.159437	O	-0.000725	0.302233	3.381390
C	1.195590	-2.671107	0.399480	O	0.000480	3.812600	-0.954366
C	1.215772	-2.581132	-1.002251	O	-0.000993	-2.822016	2.500624
C	0.001160	-2.675308	-1.765165	O	-1.510627	0.510320	-1.881872
H	4.820888	-2.250630	-0.356872	O	-6.147080	-0.467630	1.045502
H	4.854275	1.822705	0.949346	O	0.002889	-2.694589	-3.073665
H	-2.153404	1.229006	2.128172	Na	-8.080119	-0.932474	1.018344
H	2.152707	1.229155	2.129032	Na	8.083122	-0.927536	1.017034
H	-2.156707	-2.681246	0.923165	Na	-1.521103	-1.258375	2.866431
H	2.155507	-2.683654	0.924979	Na	1.518932	-1.259523	2.869612
C	-2.526285	2.613534	-0.159461	Na	-0.005062	5.696644	-0.149243
H	-2.287929	3.106854	-1.108857	Na	-0.000555	2.105891	-2.285421
H	-3.209327	3.289230	0.377142	Na	0.002707	-0.577344	-3.211500
C	2.514651	-2.240680	-1.731583	Na	-0.002646	-0.193161	-0.281781

Table S2. Summary of electronic and thermal free energies (Hartree) of optimized structures calculated at the RB3LYP/6-31G(d) level.

Compound	C4Q	Na	Na_8C4Q
$G_m^{\ominus}$(Hartree)	-1677.980750[6]	-162.27988	-2976.89008
${}^{a}E^{\ominus}$(V)		**2.280**	

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