Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

First principles study of triazine-based covalent organic framework as a high capacity anode material for Na/K-ion batteries

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Table S1. Two different stacking patterns with the same bilayer TCOF formula and their relative energy.

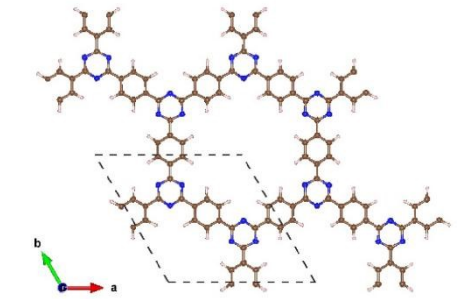
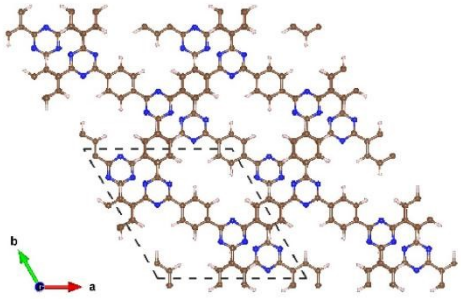
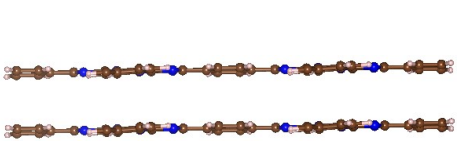
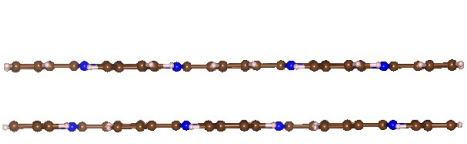
Top view		
Side view		
Stacking patterns	AA	AB
Relative energy (eV)	0	17.13

Table S2. Adsorption energies for Na/K at different adsorption sites on bilayer TCOF.

System	Adsorption energy(eV)								
	I_{H-H}	I_{TN}	I_{TC}	I_{BC}	I_B	I_T	T_{H-H}	T_B	T_T
Na-TCOF-AA	-1.259	-1.243	-1.253	-0.795	-0.773	-0.311	-0.558	-0.284	-0.039
K-TCOF-AA	-1.283	-1.273	-1.070	-0.963	-0.662	-0.378	-0.710	-0.570	-0.473

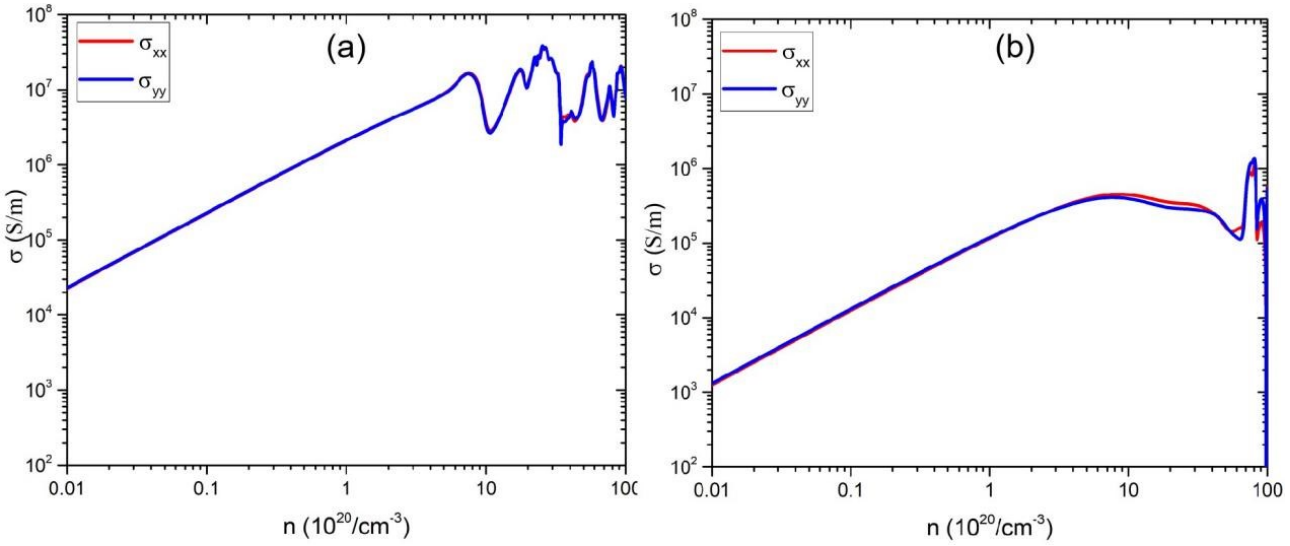


Figure S1. The electronic conductivity of the bilayer TCOF. (a) N-type and (b) P-type.

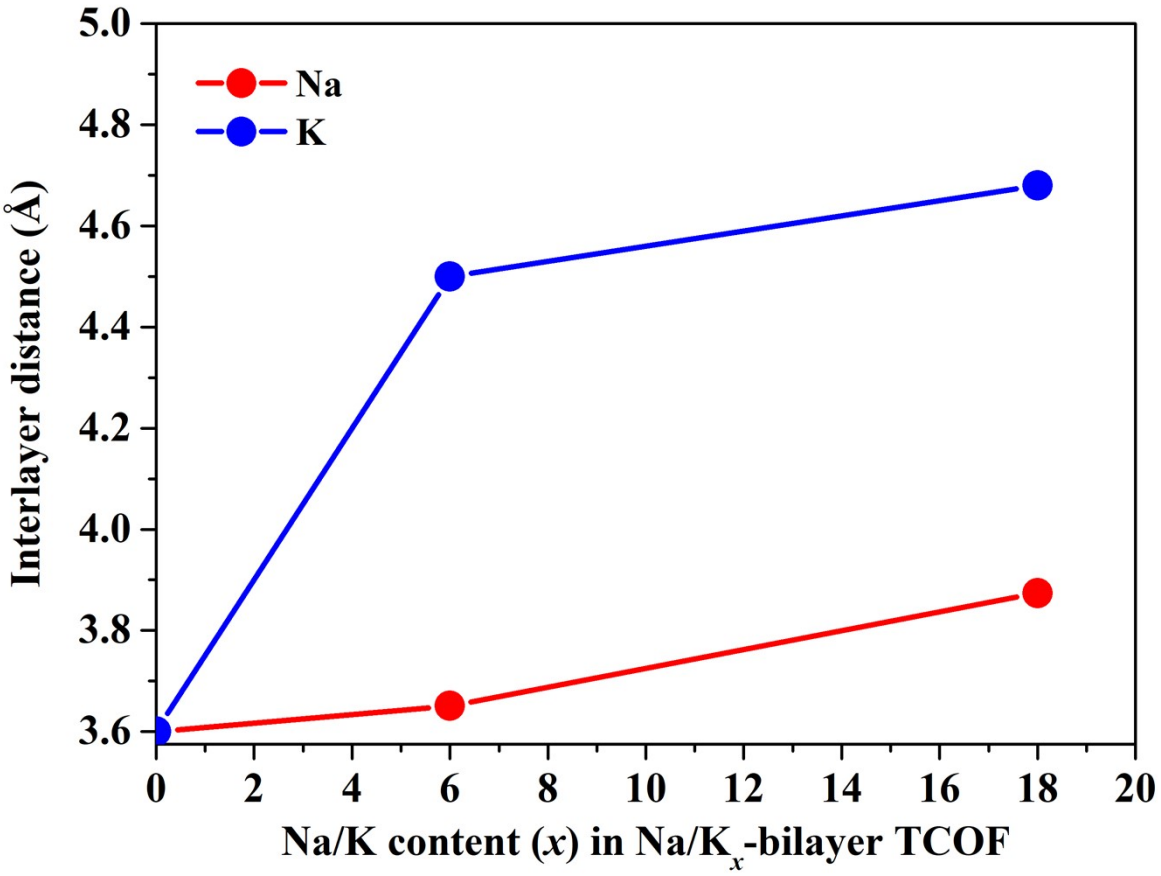


Figure S2. Interlayer distance profile diagram as a function of Na/K content (x) in the Na/K_x-bilayer TCOF.

Table S3. Diffusion barriers, theoretical capacities and Open-circuit voltages of different 2D anode materials

Anode materials	Diffusion barrier (eV)		Theoretical capacity (mAh/g)		Open-circuit voltage (V)		Ref
	Na	K	Na	K	Na	K	
TCOF	0.45	0.26	628	628	0.24	0.19	
Bi-C	0.217/0.169	0.179/0.136	485	364	0.24	0.32	[1]
β-In_2Se_3	0.14	0.09	230	230	0.03	0.13	[2]
B_7N_5	0.13	0.10	367.9	1471.5	0.22	0.14	[3]
BP	0.217	0.155	143	570	-	-	[4]
B_2S	0.19	0.04	998	499	0.06	0.18	[5]
GeS	0.090	0.050	512	256	0.13	0.33	[6]
Mo_2CrC_2	0.027	0.021	297.91	154.88	-	-	[7]
Ti_3C_2	0.096	0.103	351.8	191.8	0.137	0.128	[8]
MnC	0.174	0.138	475	235	-	-	[9]
Mo_2C	0.019	0.015	263	263	-	-	[10]
MoN_2	0.56	0.49	864	432	-	-	[11]
Si_3C	0.34	0.18	1115	836	-	-	[12]

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