batteries

Supporting Information

Titanium activation in Prussian Blue based electrodes for Na-ion batteries: synthesis and electrochemical study

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The morphology features of the as-prepared TiHCF sample are shown in figure S1 (a) and (b). As indicated by XPRD data, the crystallinity of the as-prepared sample is not high, thus, not perfect cubic morphology was found here. All of the small particles are aggregated together and exhibited various shapes, as summarized in table S1, the mean size (diameter) is around 50.3 nm.

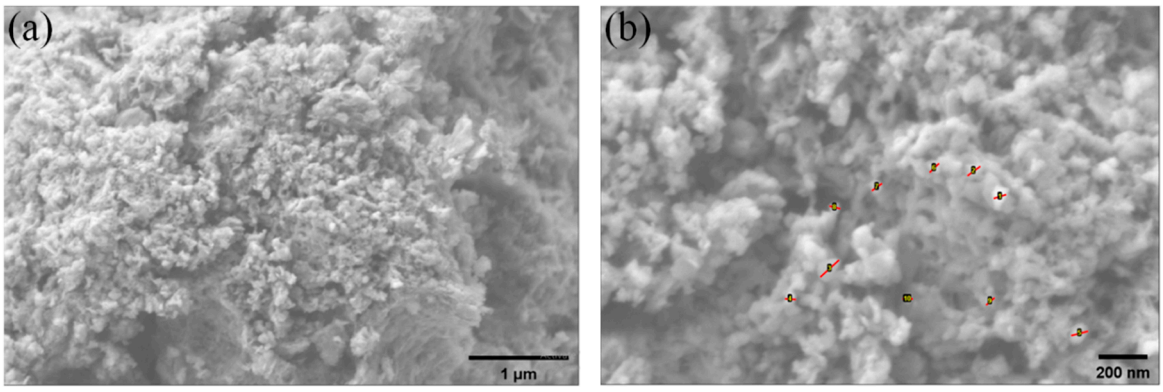

Figure S1. SEM image of TiHCF in different scales: (a) 1µm and (b) 200 nm.

Table S1. Particle size measurement (10 sites) inside Figure S1 (b).

Numbers	1	2	3	4	5	6	7	8	9	10	Mean
Sized(nm)	46.6	57.6	95.0	38.0	64.5	45.8	43.4	39.0	38.0	34.6	50.3

Details of the EXAFS analysis.

Figure S2 shows the individual EXAFS contributions, in terms of two-body, three-body, and four-body signals, to the total theoretical signal. In term of single contributions to the theoretical signals, the comparison of the total theoretical signal with the experimental, it demonstrated the reliability of this data analysis. In particular, the signals are due to the different atomic shells above mentioned, the Ti-N first shell, the Ti-N-C second shell, and the Ti-N-C-Fe third shell. All the atomic contributions herein reported are significant in the determination of the experimental signal and particular emphasis should be given to the four-body contribution (third shell) due to the metal, i.e. Fe atom (by the Ti-N-C-Fe linear chain) is of fundamental importance since it modulates the total EXAFS signal. The best fit has been obtained with E value of 4973.6(6) eV, which is displaced by several eV in respect to the edge inflection point. The value of S02 was found to be 0.65(5). The atomic distances related to the Fe-C-N-Ti linear chain, i.e., the Fe-C, C-N, and Ti-N distances, have been found to be 1.87(2), 1.18(2) and 2.07(9) Å respectively, in good agreement to those of similar metal hexacyanoferrate material.

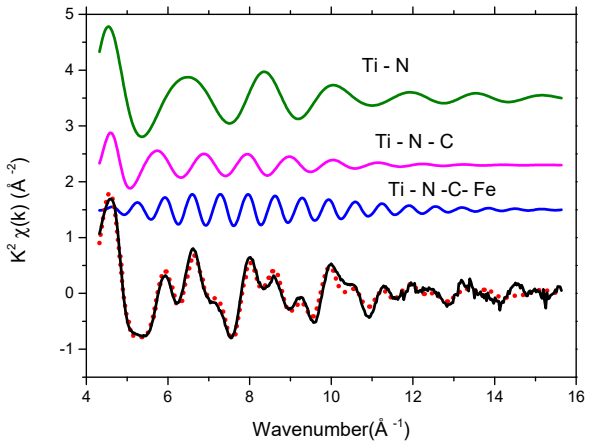

Figure S2. Details of the EXAFS analysis of the Ti K-edge of TiHCF, the comparison of the total theoretical signal (red) with the experimental one (black).

Further details of the galvanostatic test at C/20.

By considering the Na-ion half cell as an example, the current was calculated based on the cathode (TiHCF pellet) mass. The theoretical capacity of the as-prepared sample is 83.6 mAh g-1 (considering 1 mol e- participating in the reaction). The mass of the pellet for the Na-ion half cell is 1.95 mg (active material 85%). Then we can get the battery capacity in mAmp-hour (mAh)=83.6*1.95*10-3*85%=0.1386 mAh. As C/20 means considering the total discharge process in 20h, then the current to be applied is 0.00693 mA. In addition, by considering the diameter of pellets 12mm, the area is 1.1304 cm2, then the current density at C/20 is 0.00613 mA/cm2. A similar calculation for the Li-ion half cell: electrode mass 1.79mg, the current is 0.00636 mA at C/20, and the current density is 0.00563 mA/cm2.