Supporting Information

Electrochemical lithium storage of a biactive organic molecule containing cyano and imine groups

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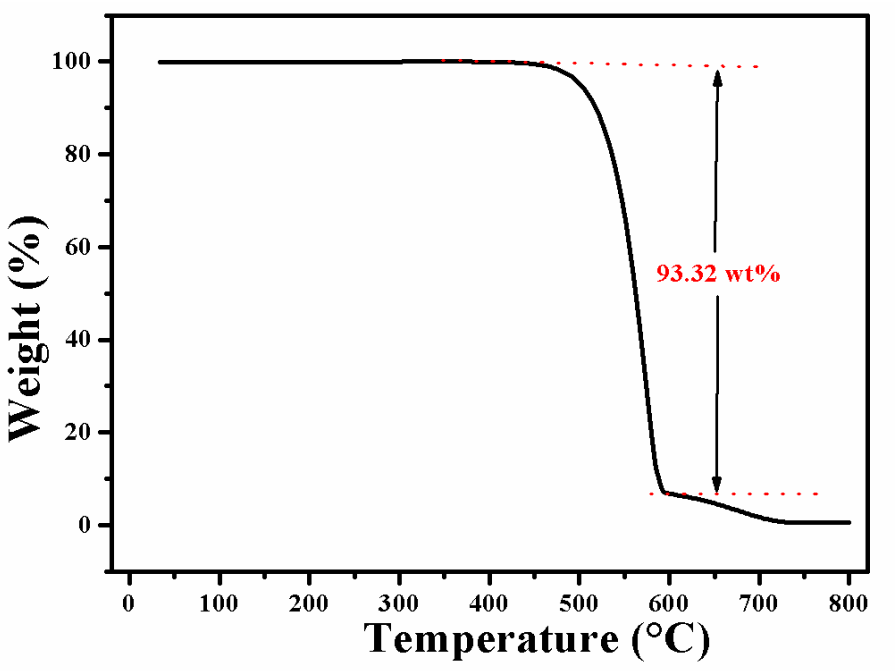


Fig. S1. TGA curves of HAT with a heating rate of 10 ^{o}C min^{-1} under air atmosphere.

The absence of significant weight loss in HAT until the temperature reached 460 °C indicates the good thermal stability of HAT up to 460 °C in air (Fig. S1).

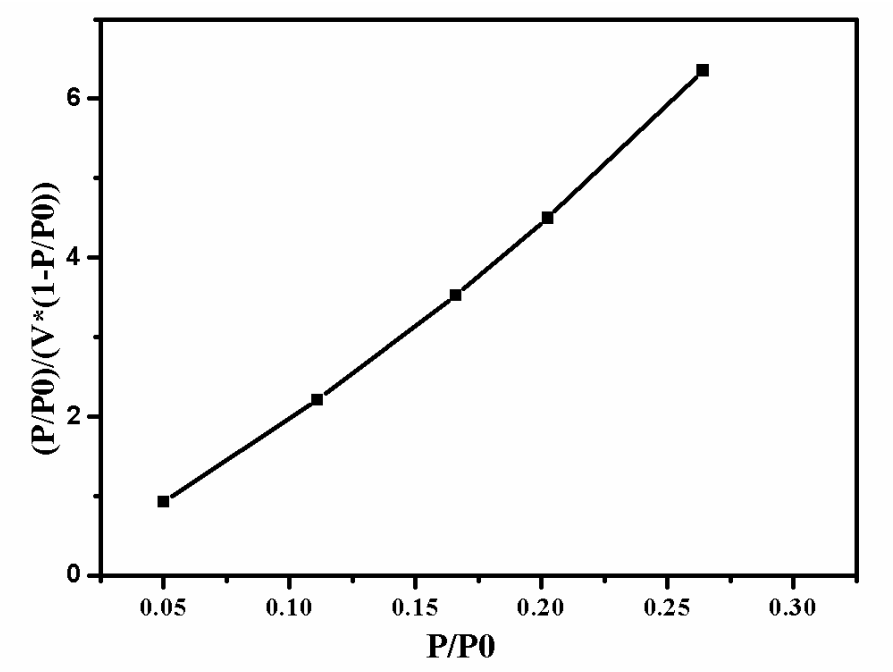


Fig. S2. BET surface area curves of HAT.

The specific surface areas of HAT is 0.051 m^2 g^{-1}.

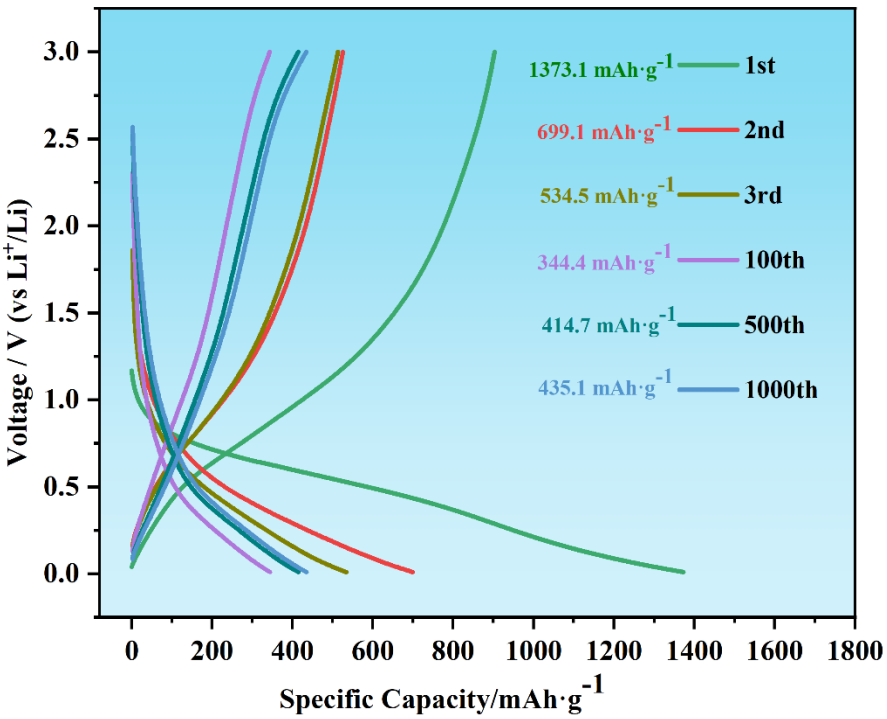


Fig. S3. Charge/discharge curves of HAT after different cycle numbers at 800 mA g^{-1}.

The galvanostatic charge and discharge curves are shown in Fig. S3 is analysed at 800 mA g^{-1}. The first charge capacities is obtained to be 1373.1 mAh g^{-1}. The specific capacity increased from 344.4 mAh g^{-1} to 435.1 mAh g^{-1} after the last 500 cycles, which could be ascribed to the reaction rate, extent and kinetics having been improved with activation through the last several cycles, and it could keep a specific capacity of 344.4 mAh g^{-1} after 100 cycles. The decay of the specific capacity may be ascribed to aggregation caused by the irreversible extent of the reaction.

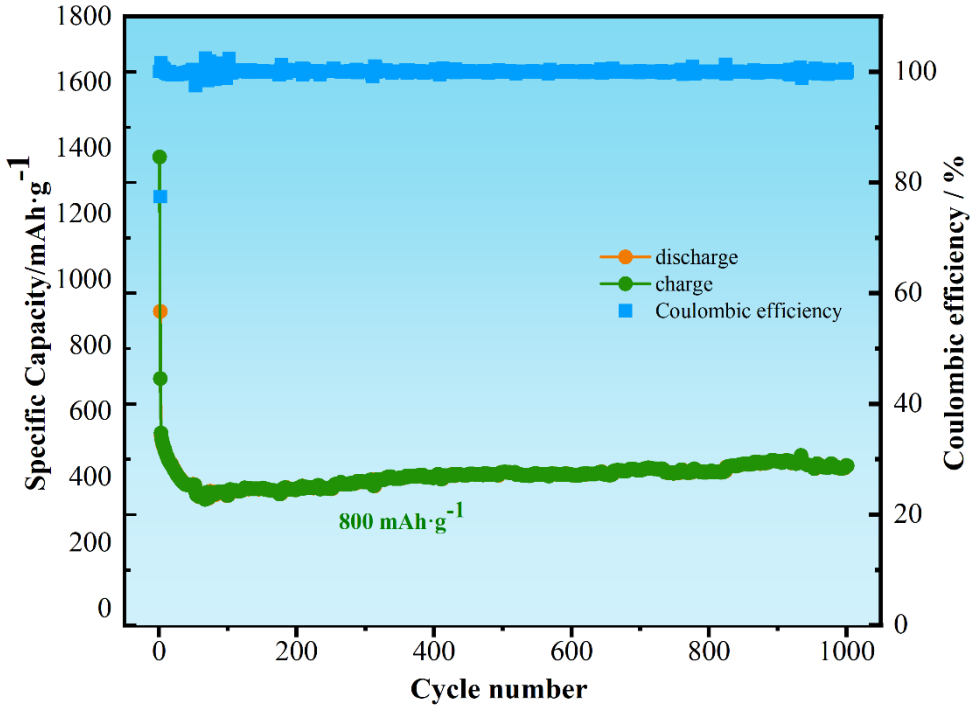


Fig. S4. Cycling and Coulombic efficiency of HAT at current density of 800 mA g^{-1}.

The second discharge capacity of HAT at 800 mA·g^{-1} was 699.1 mAh g^{-1}, and a reversible capacity of 435.1 mAh g^{-1} was maintained after 1000 cycles, indicating a fairly small increase.

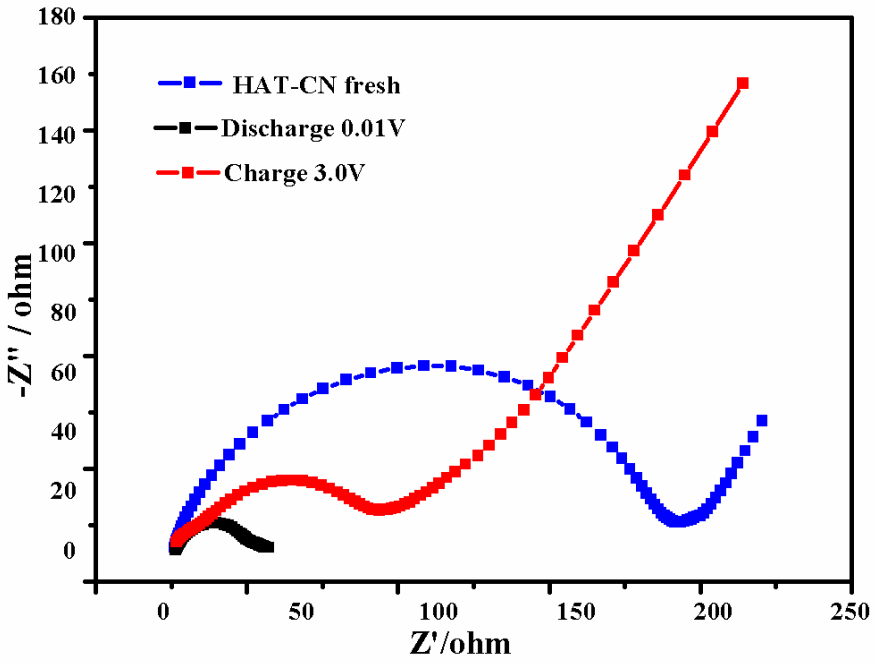
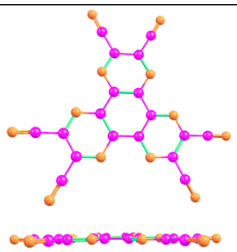
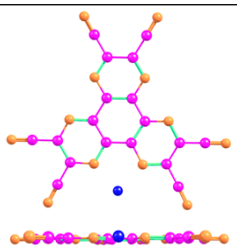
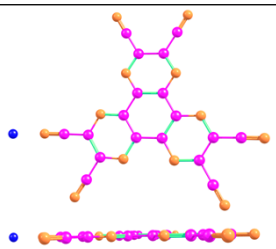
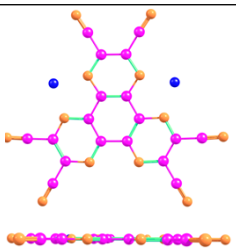
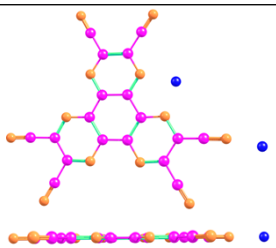
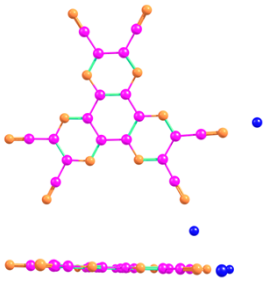
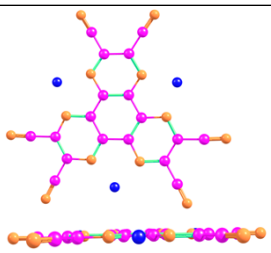
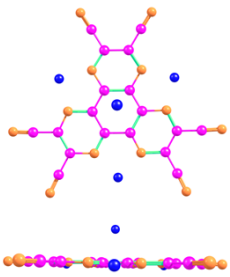
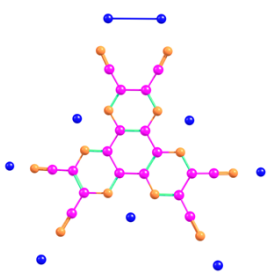


Fig. S5. The EIS comparison of HAT at different states.

The in-situ impedance of the HAT, fresh HAT, HAT discharged to 0.01V and recharged to 3 V, respectively as shown Fig. S3. It can be seen from this figure that the in-situ impedance of the HAT is 186.50 Ω; when discharged to 0.01 V, the impedance is 37.40 Ω, and when recharged to 3 V, the impedance is 78.50 Ω. It shows that the resistances of the first and second times are quite different, that is, the first irreversible capacity loss of the battery is larger. This shows that the intercalated lithium cannot be fully extracted, and the diffusion capacity is weakened.

HAT			
ΔE/kcal			
HAT-1Li			
ΔE/kca	**-65.10097**	-53.45440	
HAT-2Li			
ΔE/kca	**-123.45622/**	-104.25443	-87.86388
HAT-3Li			
ΔE/kca	-189.56748		
HAT-4Li			
ΔE/kca	-210.1466		
HAT-9Li			

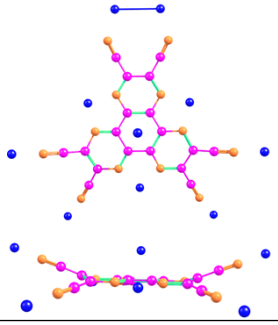
			
ΔE/kca	-272.76897		
HAT-10Li			
ΔE/kca	-276.05398		

Fig. S6. Possible structure and theoretical calculation energy proposed in the process of HAT lithiation: HAT, HAT+1Li, HAT+2Li, HAT+3Li, HAT+4Li, HAT+9Li, and HAT+10Li.

To further explore the storage mechanism of HAT anode in the LIB, DFT calculations were performed to simulate the lithiation process of HAT. The optimized structures of HAT and HAT +Lin (n = 0, 1, 2, 3, 4, 9, 10) and their respective total energy energies were calculated. As shown in Fig. S4. From the HOMO-LUMO energy level difference of unconnected Li^+, connected $3Li^+$ and connected $9Li^+$, it can be seen that the energy band gap is continuously decreasing. Combining with the Fig. 3, the planar structure formed by HAT+Li3 had the smallest LUMO−HOMO band gap (ΔE = 1.16 eV). The band gap usually refers to the energy difference between the top of the valence band and the bottom of the conduction band, which is the main factor determining the electrical conductivity of a material.