Supporting materials

Low Temperature Carbonization of Cellulose Nanocrystals for High Performance Carbon Anode of Sodium-Ion Batteries

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Supporting Figures

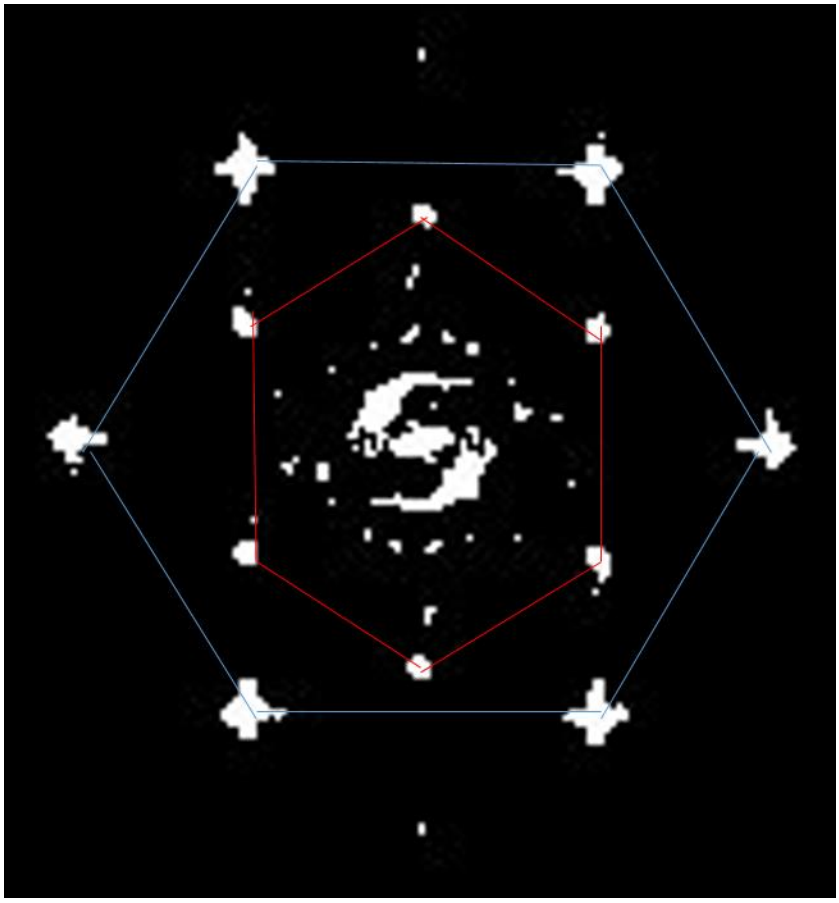


Figure S1 Thresholded FFT Analysis of HRTEM (Figure 1b). Lines connecting the dots are added to demonstrate the hexagonal pattern. The blue hexagon corresponds to hexagonal pattern at 1.42 Å, while the red one corresponds to hexagonal pattern at 2.21 Å.

To measure the resistivity of carbonized CNC, an Agilent B2901A tester was used. The setup is shown in Figure S2. The thickness of the carbonized CNC sample used here is 0.035 mm, while the distance S between probes is 1.59 mm. When applying a 10 mA current, the V_{23} is measured to be 81.7 mV. The resistivity is calculated to be 0.13 Ω·cm.

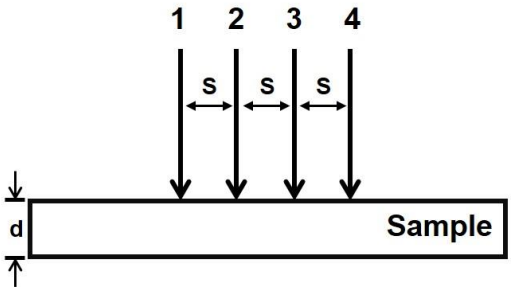
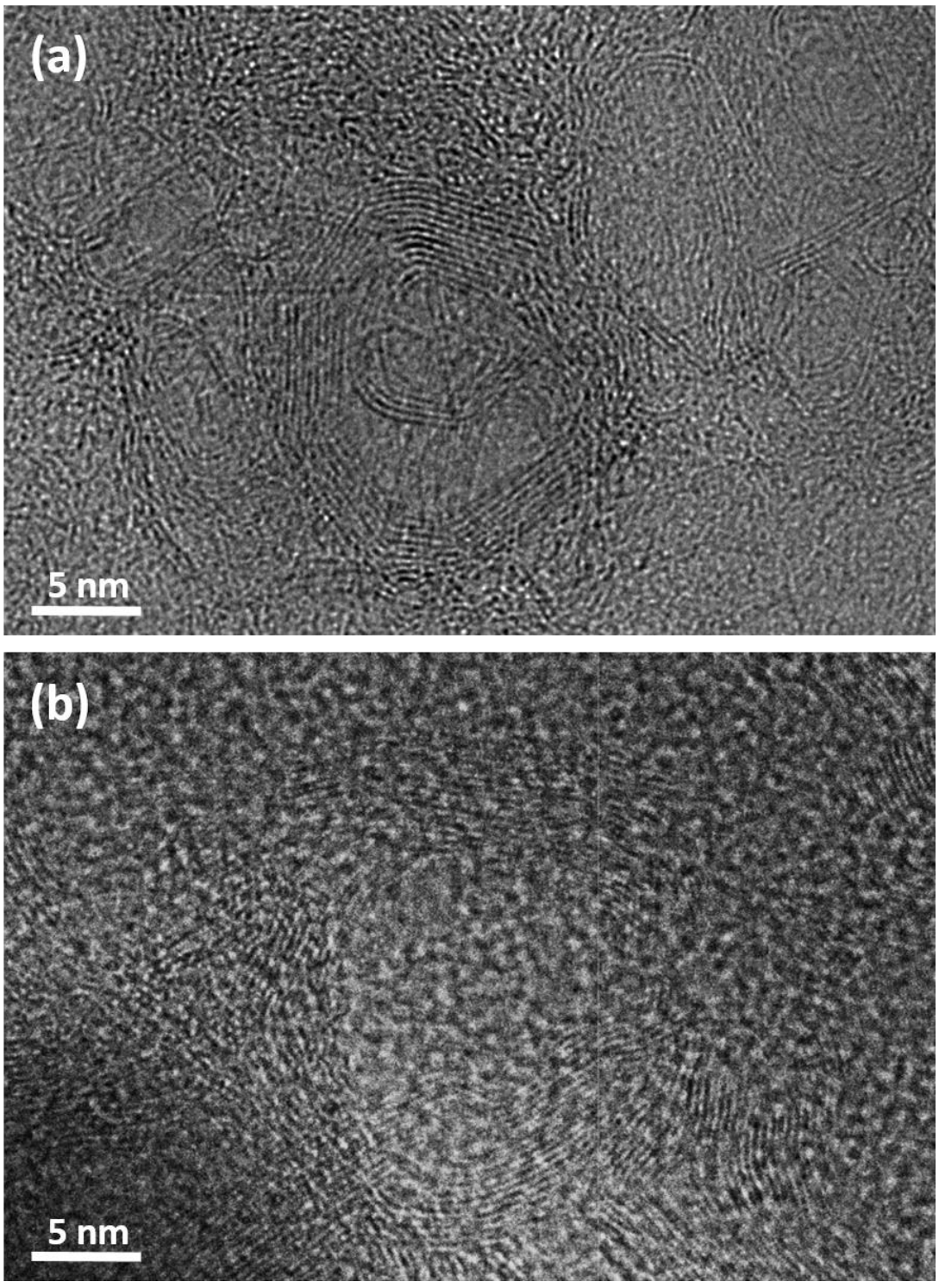


Figure S2. Schematic for four-probe setup to measure conductivity.


(a)
5 nm
(b)
5 nm

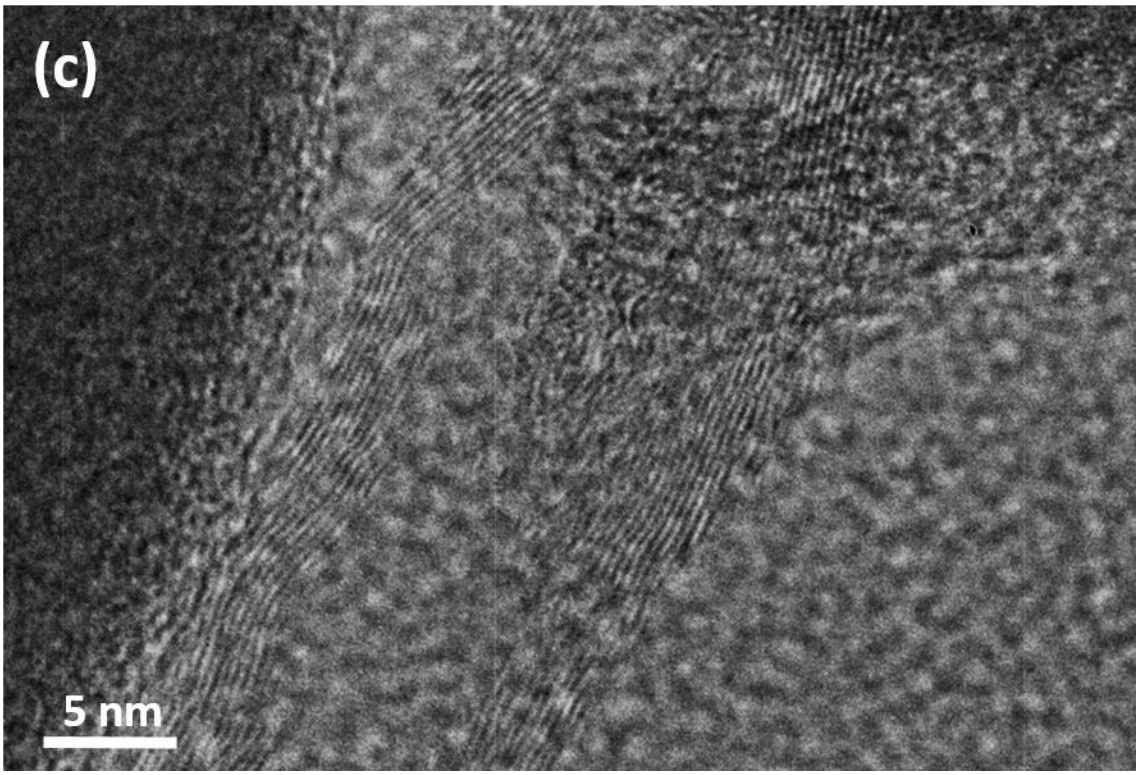


Figure S3. Local ordered nanocarbon in carbonized CNC at 1000°C. (a-c) HRTEM images of carbonized CNC.

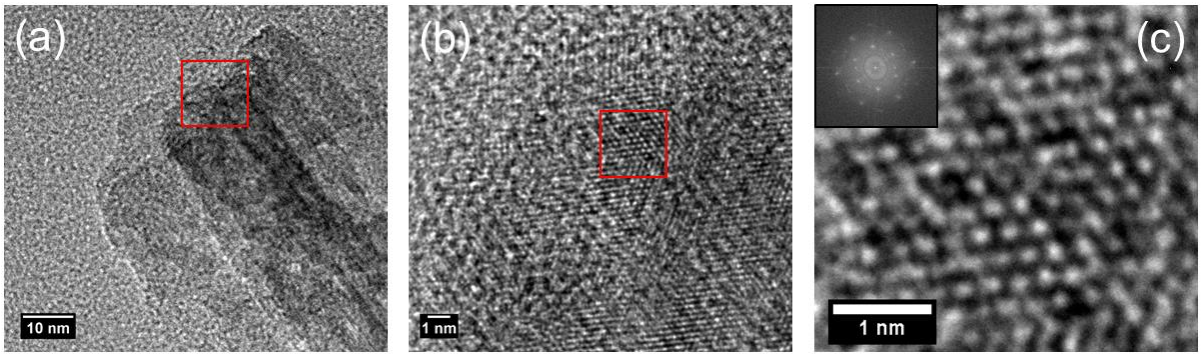


Figure S4. Hexagonal structures observed in carbonized CNC at 1000°C. (a) TEM of the obtained carbon; (b) HRTEM of the area contained in the red square of (a); (c) Higher magnification of the area contained in the red square in (b), inset shown the Fourier transform.

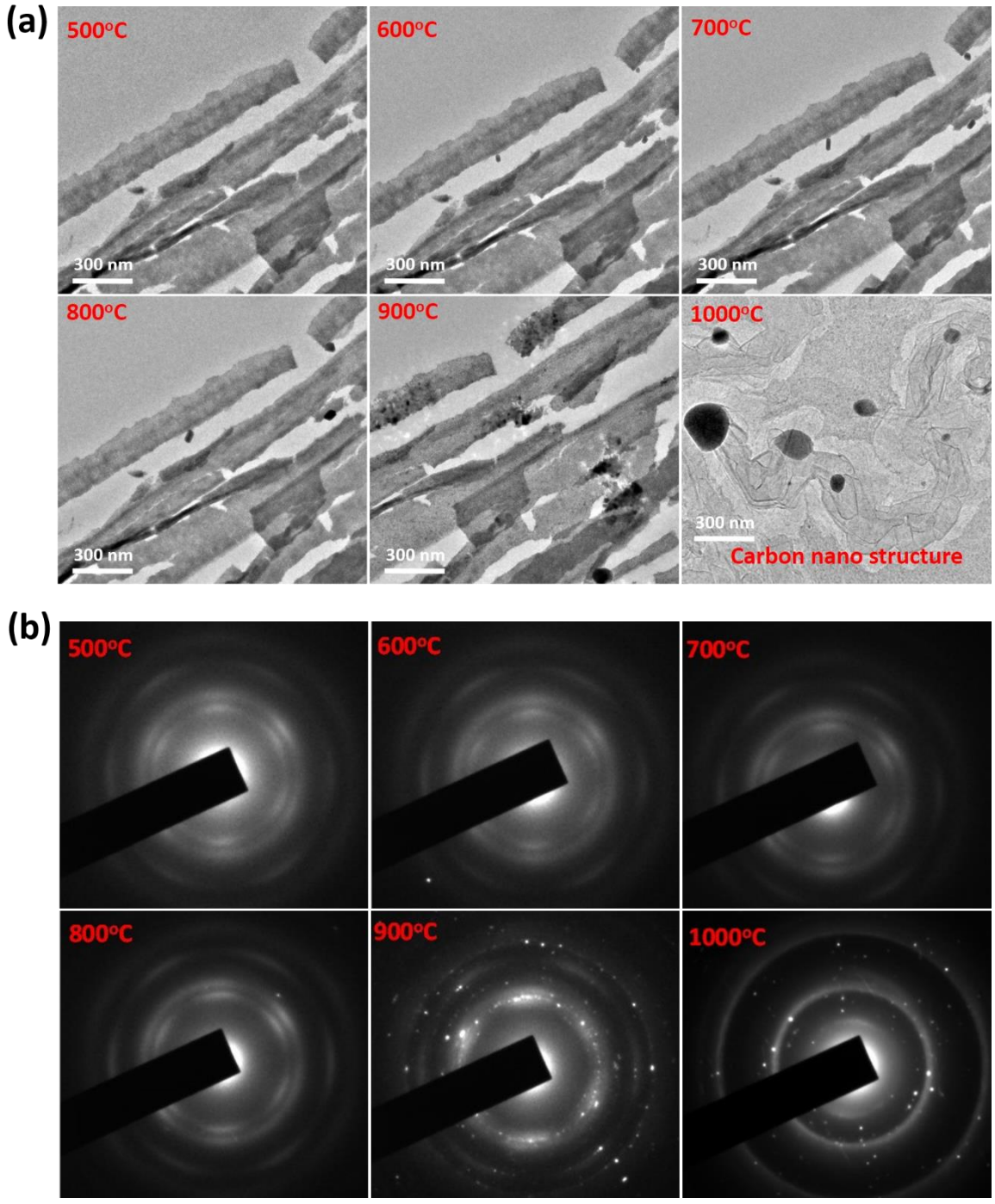


Figure S5. *In-situ* TEM characterization of CNC carbonization process from 500 to 1000 °C. (a) TEM images at different temperatures and (b) corresponding diffraction patterns.

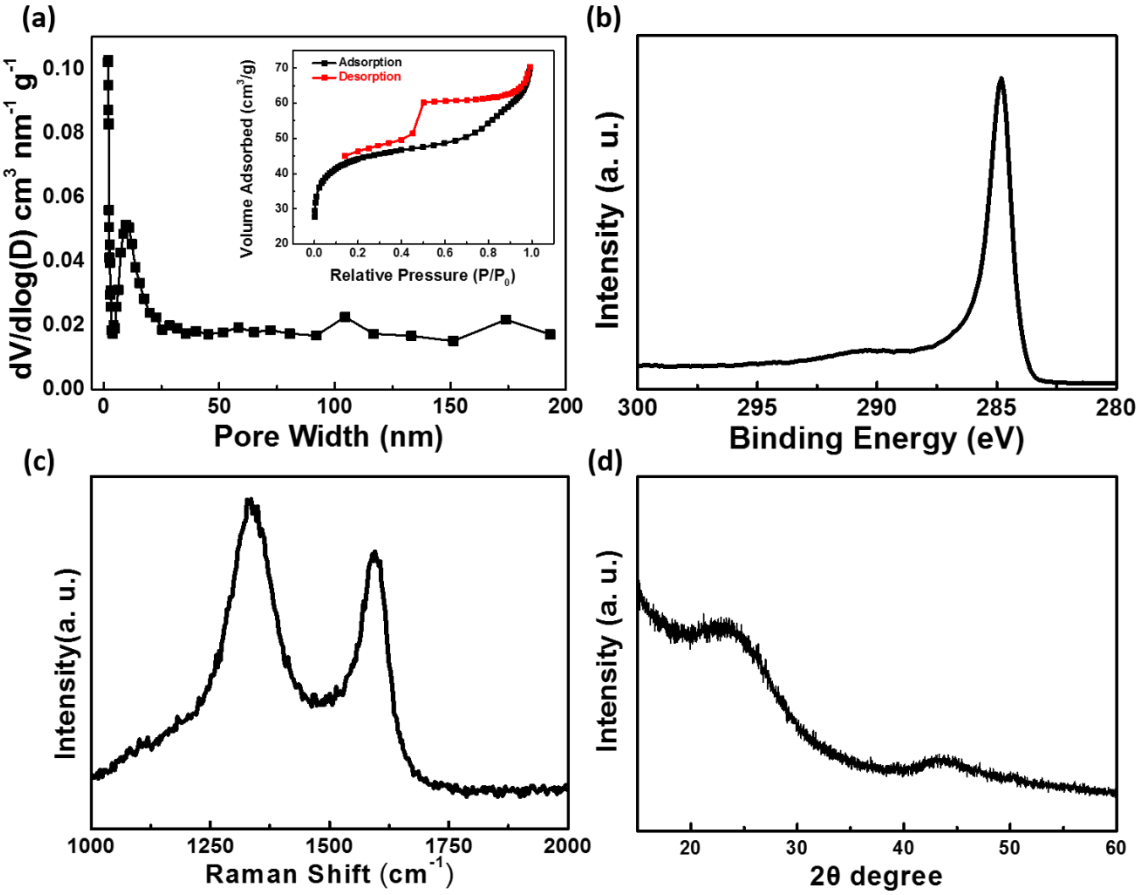


Figure S6. Characterization of carbonized CNC: (a) Pore size distribution (calculated from the adsorption isotherms using the BJH method) with the inset showing nitrogen adsorption/desorption isotherms; (b) Survey XPS spectrum, (c) Raman spectra and (d) XRD pattern.

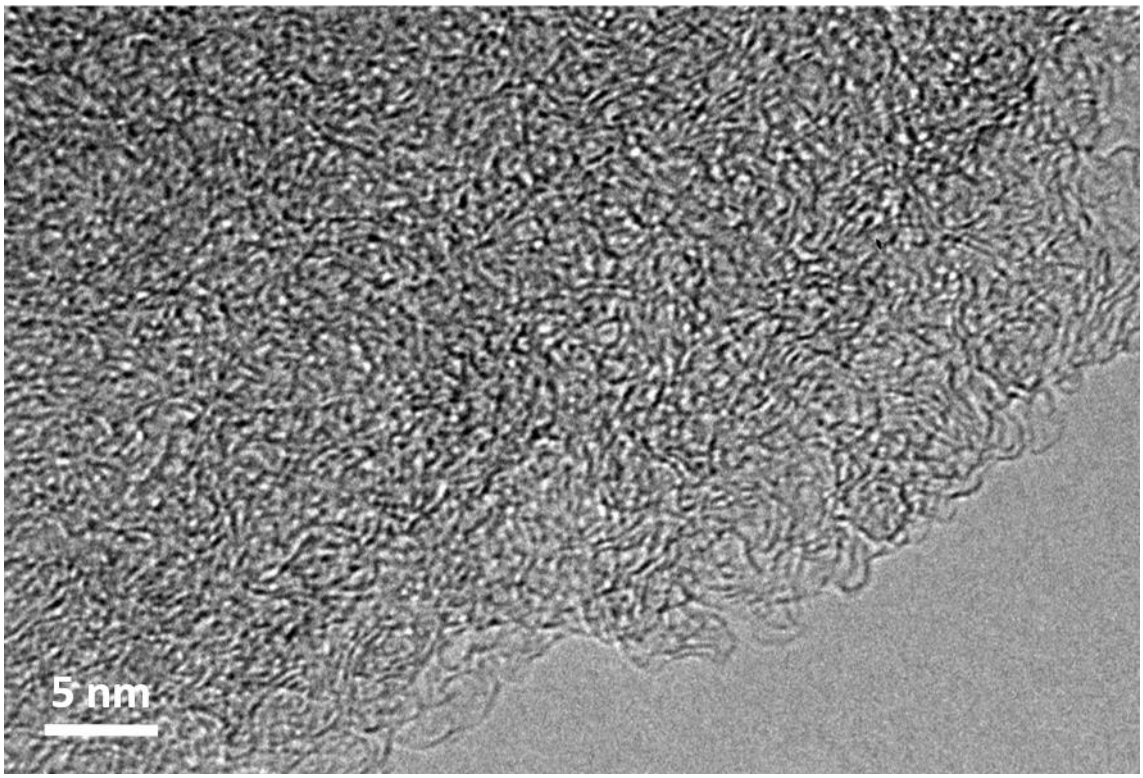


Figure S7. HRTEM image of carbonized regular cellulose fiber.

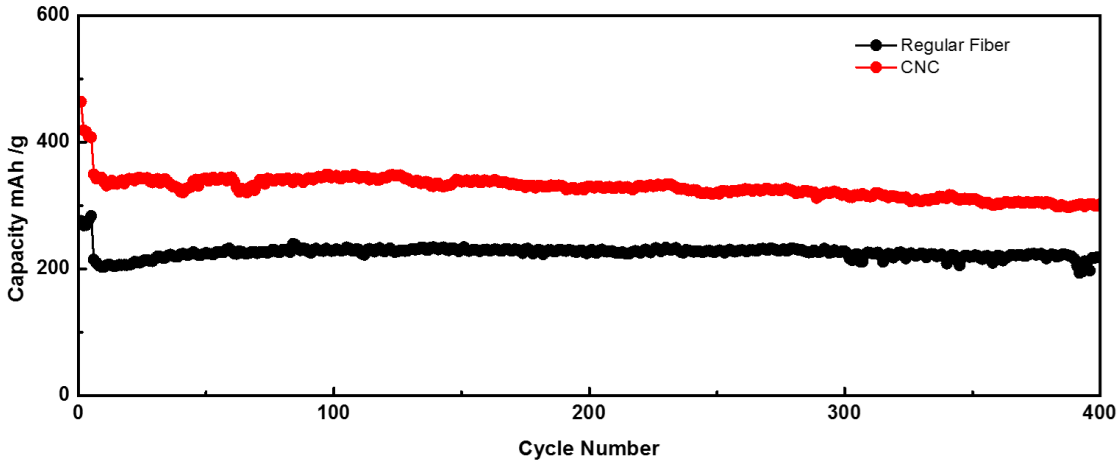


Figure S8. Cycling performance of carbonized regular cellulose fiber (black symbol) and carbonized CNC (red symbol).

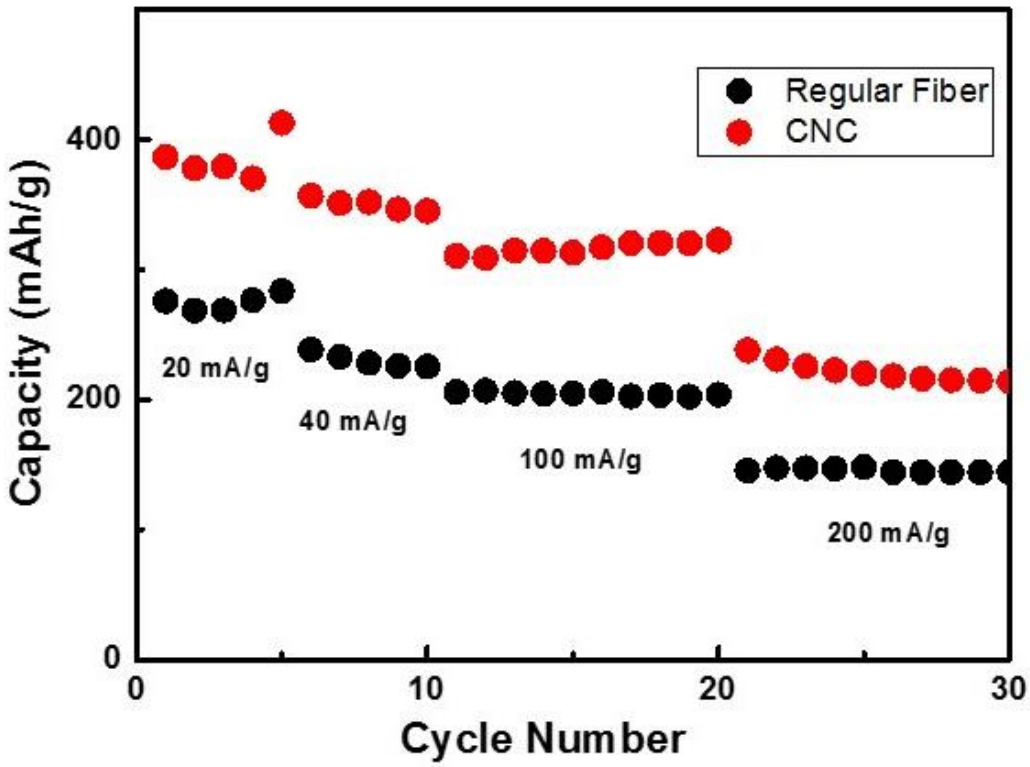


Figure S9. Compare of rate performances of carbonized regular cellulose fiber (black symbol) and carbonized CNC (red symbol).

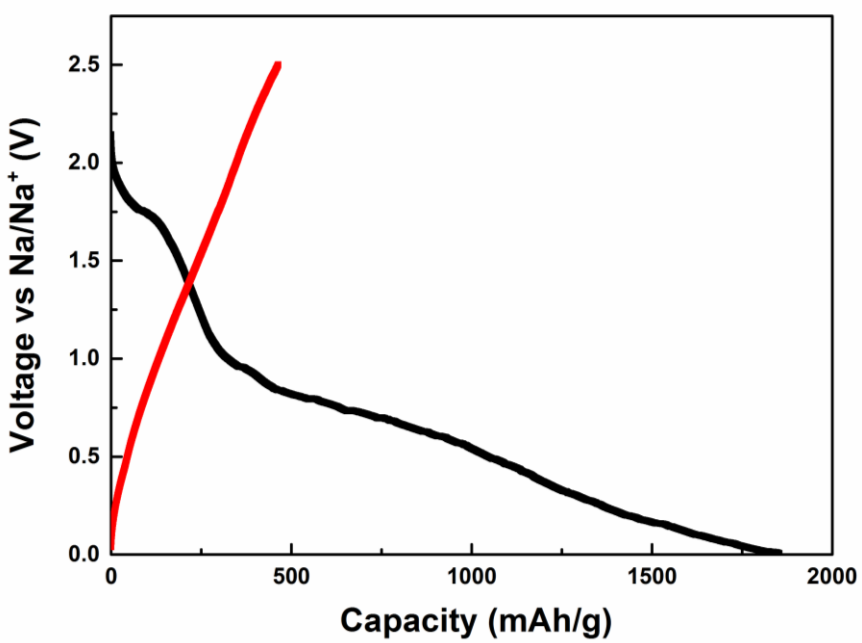


Figure S10. Initial charge/discharge profiles of carbonized CNC at a current density of 10 mA/g.

Simulation method in detail

Our full atomistic simulation study employs the ReaxFF potential and simulation is carried out using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The simulation is subjected to a NVT ensemble. The time step is set to 0.5 femtoseconds (fs). The thermostat is Nose-Hoover style and the temperature is relaxed every 0.5 ps. The simulation for thermal decomposition (Figure 4(e) to 4(h)) is carried out at a step-wise temperature profile. The temperature difference between neighboring steps is set to 100K. During each temperature step, the system is equilibrated for 75 ps. For example, the system is equilibrated in 300K, for 75 ps and then the temperature is increased to 400K, for another 75 ps. The simulation for formation of graphene-like structures (Figure 4(i) to 4(l)) is carried out at 1300K. Carbon radicals generated from the thermal decomposition is constantly shuttled into a planar periodical simulation box with constantly decreasing sizes, in an effort to simulate the increasing spatial density of the carbon radicals in the system.