Solution-Phase Synthesis of Heteroatom-Substituted Carbon Scaffolds for Hydrogen Storage—Supporting Information

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<u>Supporting Information including:</u>

S1. HRTEM images of pristine carbon scaffolds

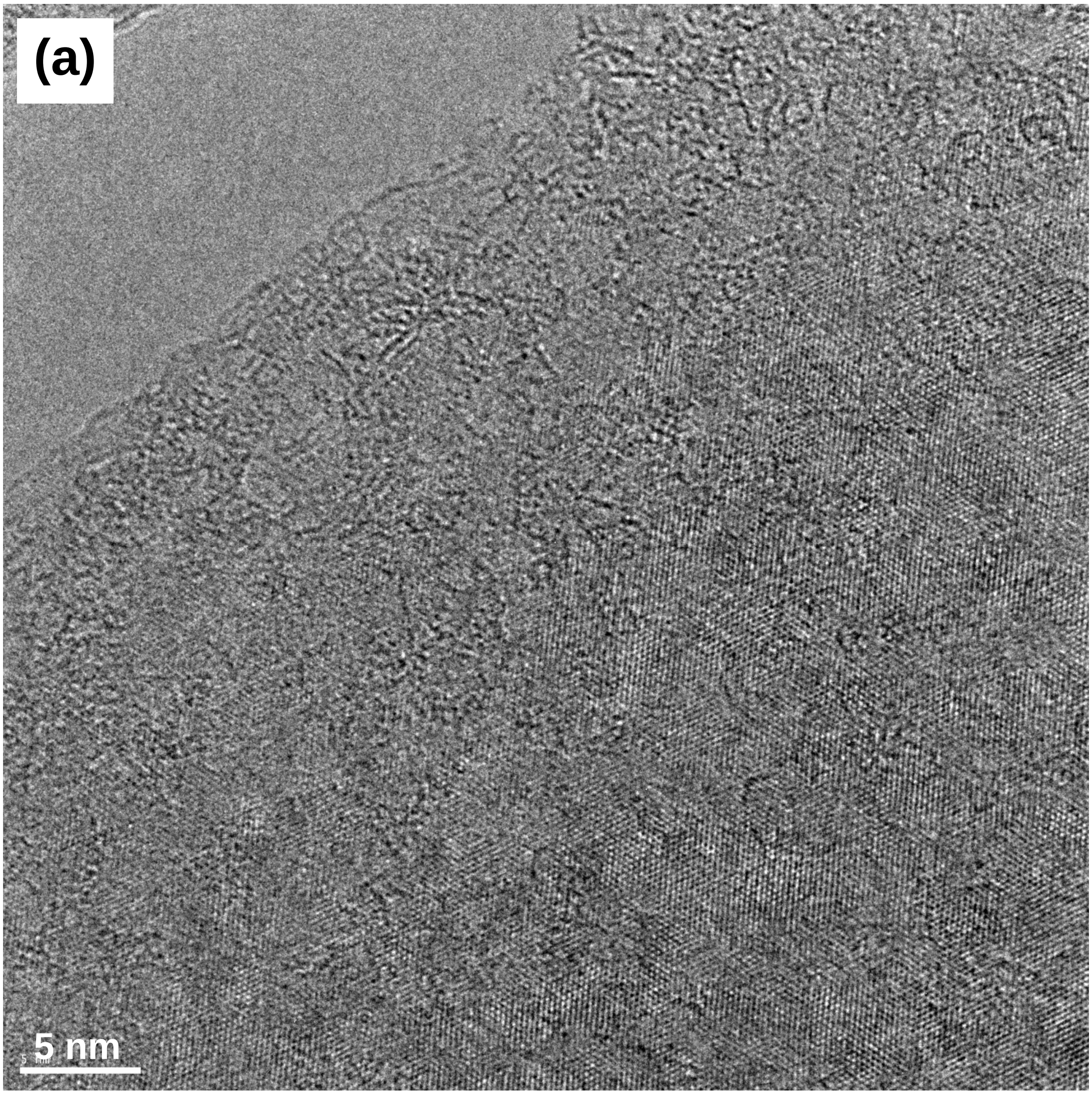
S2. XPS survey scans of pristine and heteroatom-substituted carbon scaffolds

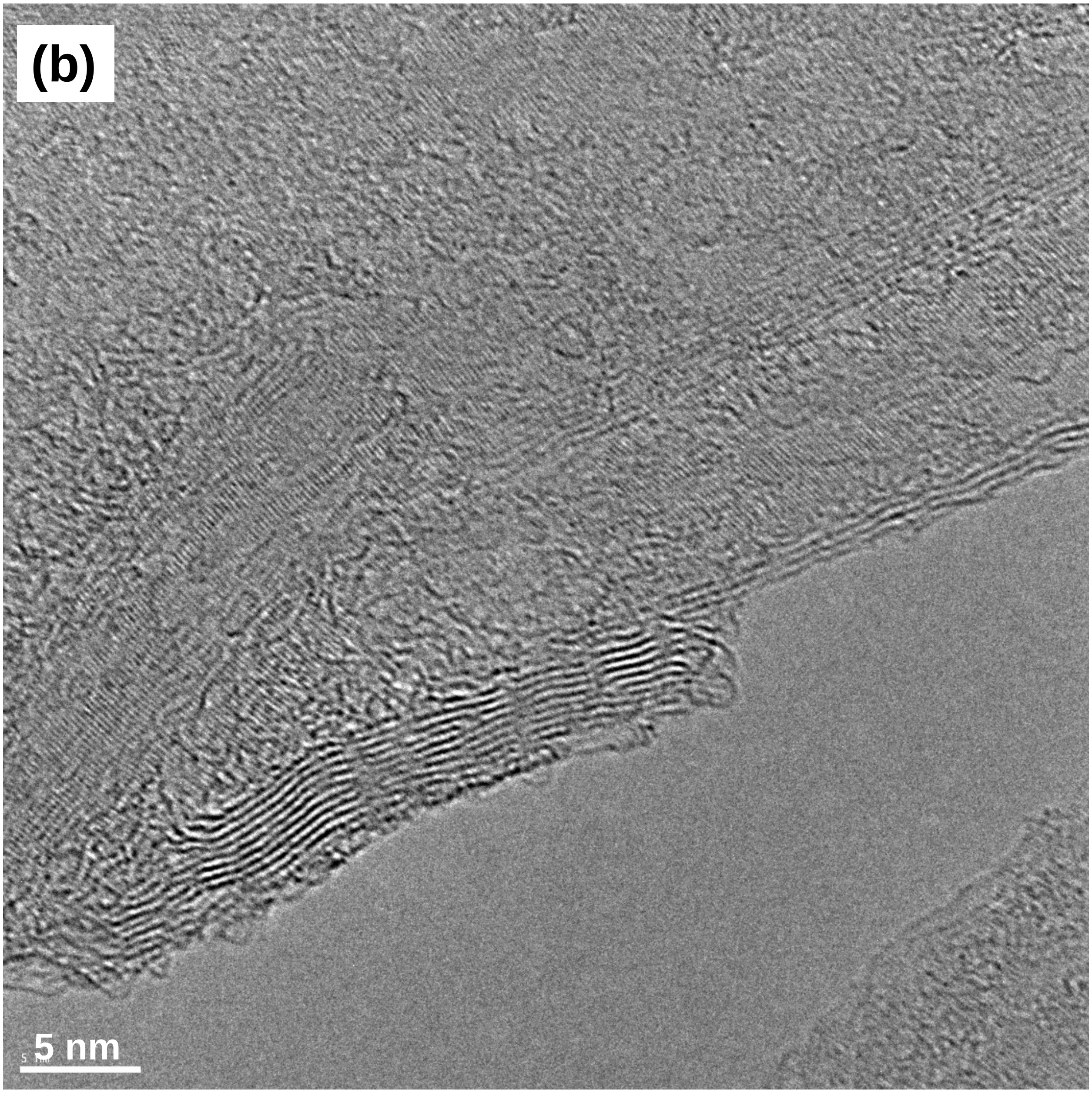
S3. EFTEM elemental mapping of heteroatom-substituted carbon scaffolds

S4. Pore size distribution of pristine and heteroatom-substituted carbon scaffolds

S1. HRTEM images of pristine carbon scaffolds

Figure S1a and S1b show graphitic micro-sheets of pristine carbon scaffold sample prepared by the bottom-up procedure. The size distribution of the graphitic micro-sheets is from several hundred nanometers to ~ 2 μm. In Figure S1a, 3-5 nm-sized micro domains of graphene nanoflakes can be observed stacked on the surface, which indicates the graphitic micro-sheets were produced from smaller graphene nanoflakes. Figure S1b shows a nanoscale fold near a region of a ridged wrinkle on the graphitic micro-sheets.




(b)
5 nm

S2. XPS survey scans of pristine and heteroatom-substituted carbon scaffolds

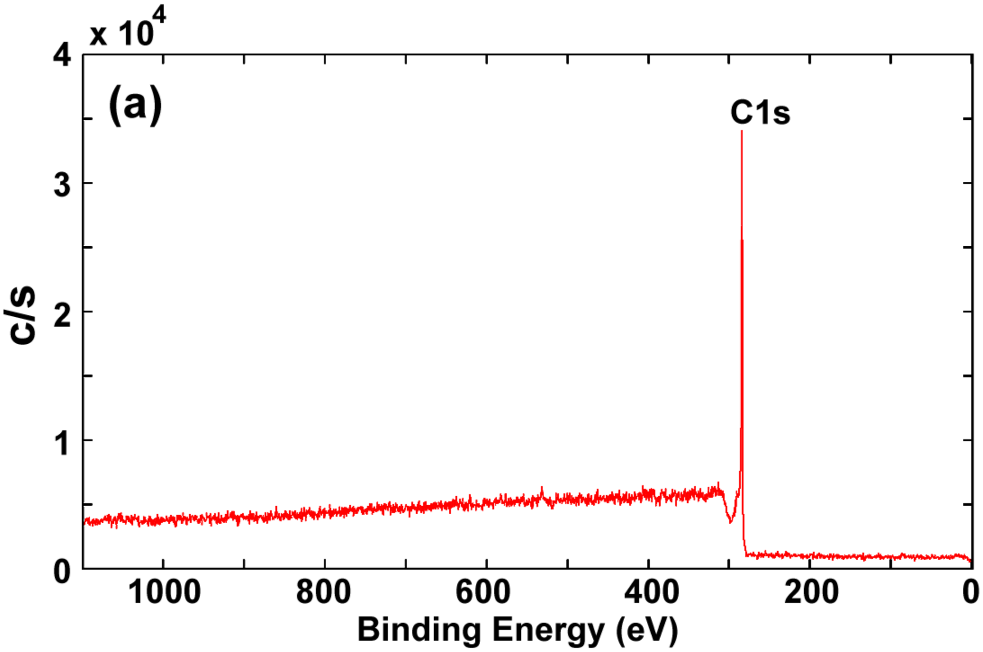


Figure S2a. XPS survey scan of pristine carbon scaffold.

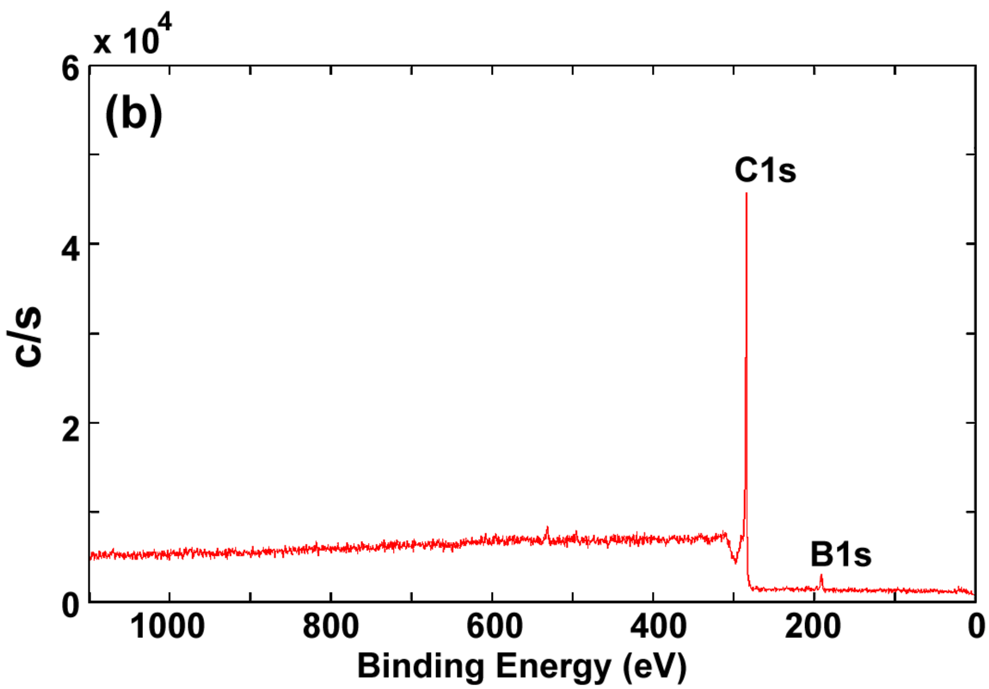


Figure S2b. XPS survey scan of boron-substituted carbon scaffold.

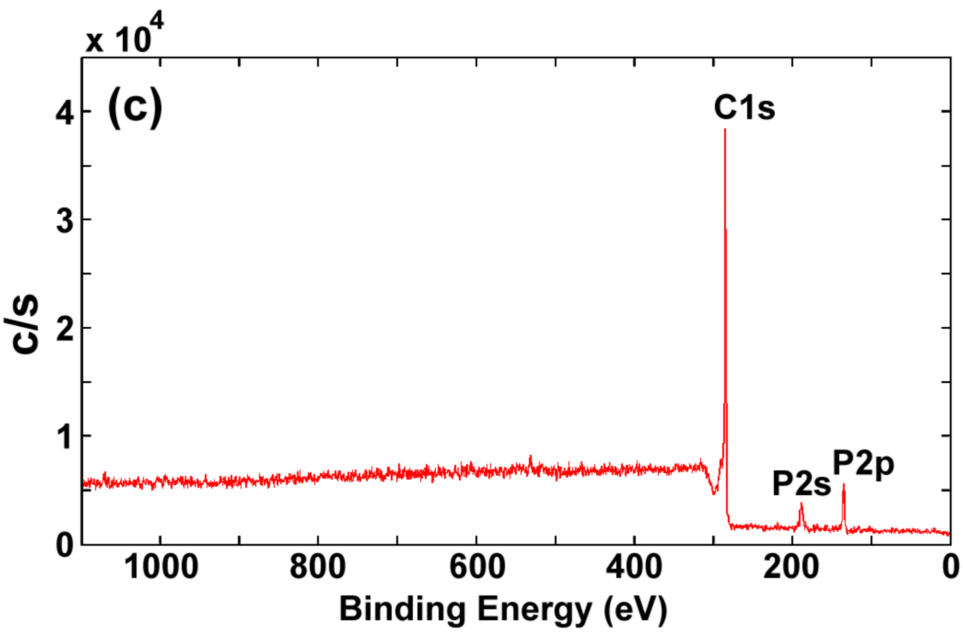


Figure S2c. XPS survey scan of phosphorous-substituted carbon scaffold.

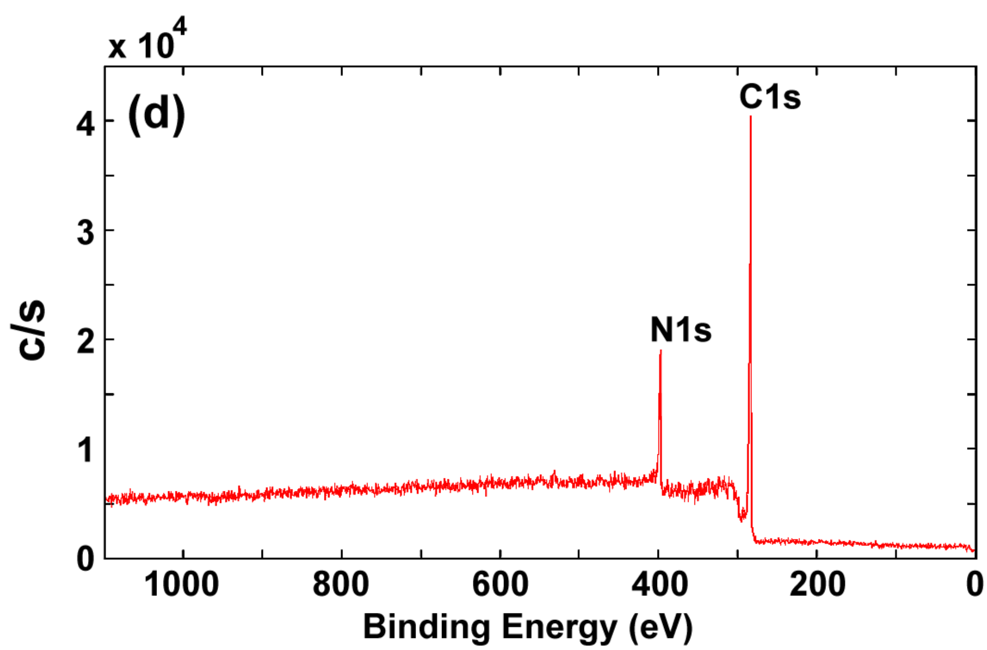


Figure S2d. XPS survey scan of nitrogen-substituted carbon scaffold.

S3. EFTEM elemental mapping of heteroatom-substituted carbon scaffolds

Figure S3a-f show TEM images (left) and EFTEM elemental mapping of carbon (middle) and substituted atoms (right) of heteroatom-substituted carbon scaffolds: boron (a, b, c) and phosphorous (d, e, f). The carbon atoms are represented by green dots, while the substituted atoms are represented by red dots.

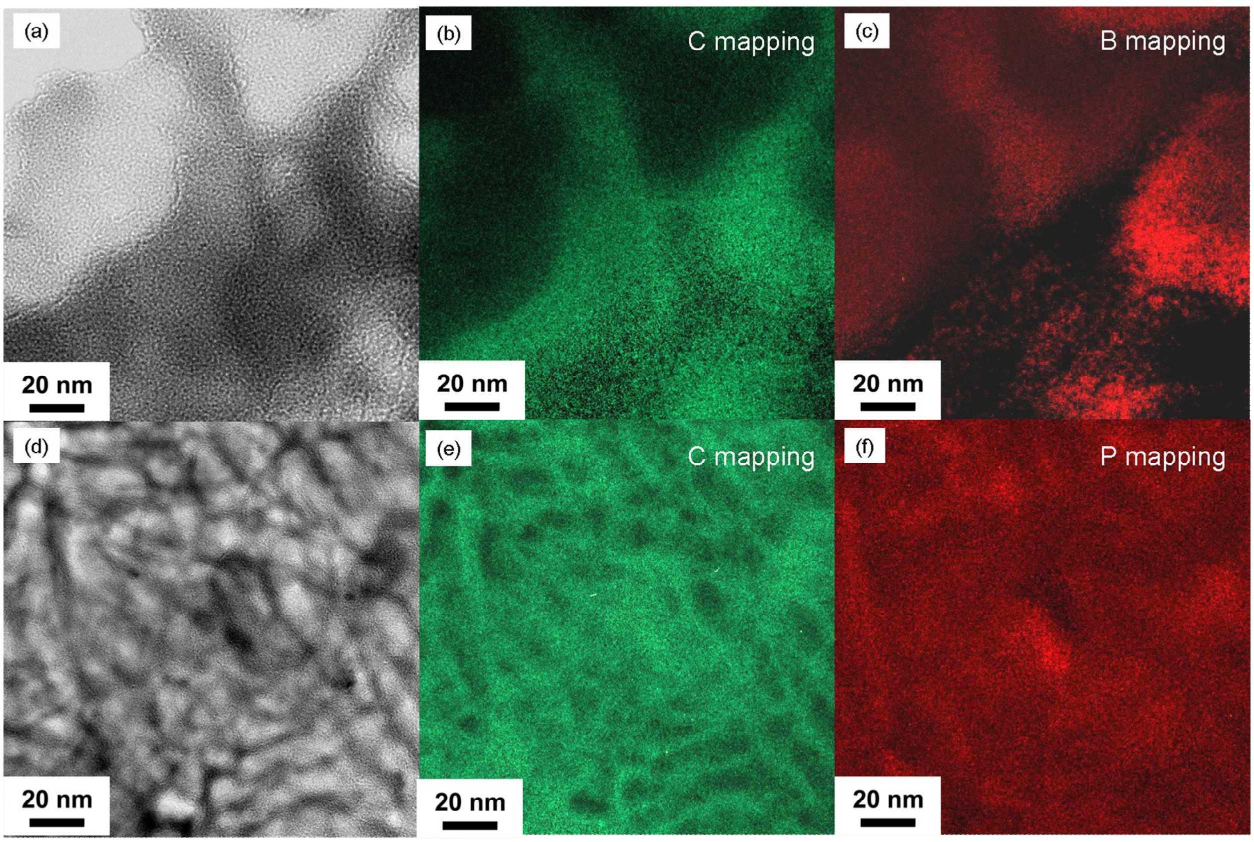
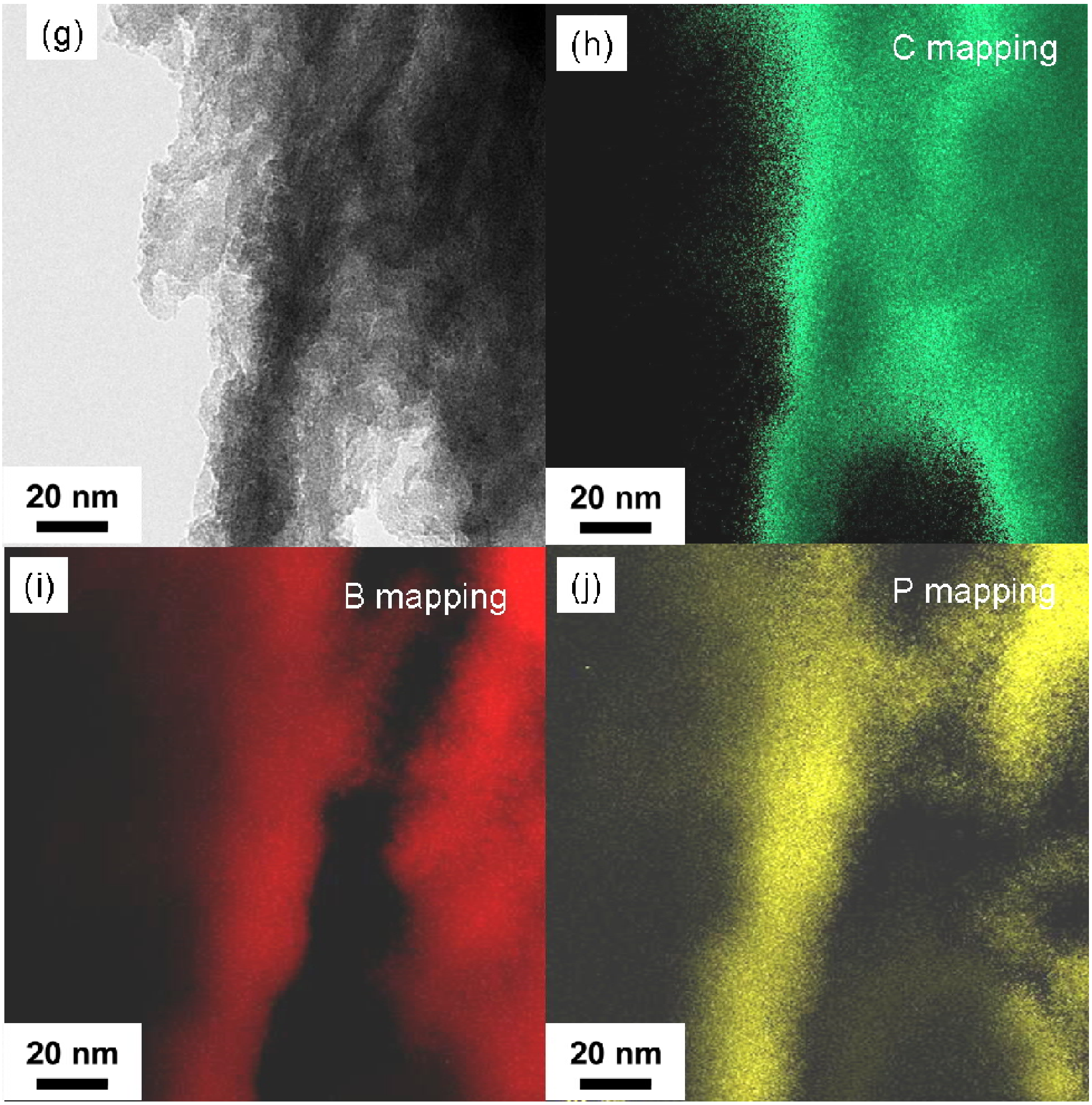


Figure S3g-j show TEM image (top left) and EFTEM elemental mapping of boron/phosphorous co-substituted carbon scaffold. Carbon atoms are still represented by green dots, boron atoms are represented by red dots, and phosphorous atoms are represented by yellow dots.



S4. Pore size distribution of pristine and heteroatom-substituted carbon scaffolds

Figure S4a-f show the pore size distribution of pristine and heteroatom-substituted carbon scaffolds calculated using the BJH (Barrett-Joyner-Halenda) method with the nitrogen BET adsorption data. All of the carbon scaffolds exhibit narrow peaks between 2.3-2.8 nm pore diameter and a shoulder peak extending to the atomic scale micropores. The values for the heteroatom-substituted carbon scaffolds are larger than the peak due to the pristine carbon scaffolds at the same range. As shown in the Figure S4d, in contrast to the pristine, boron- or phosphorous-substituted carbon scaffolds, the nitrogen-substituted carbon scaffolds have only a small shoulder peak extending to the atomic scale micropores.

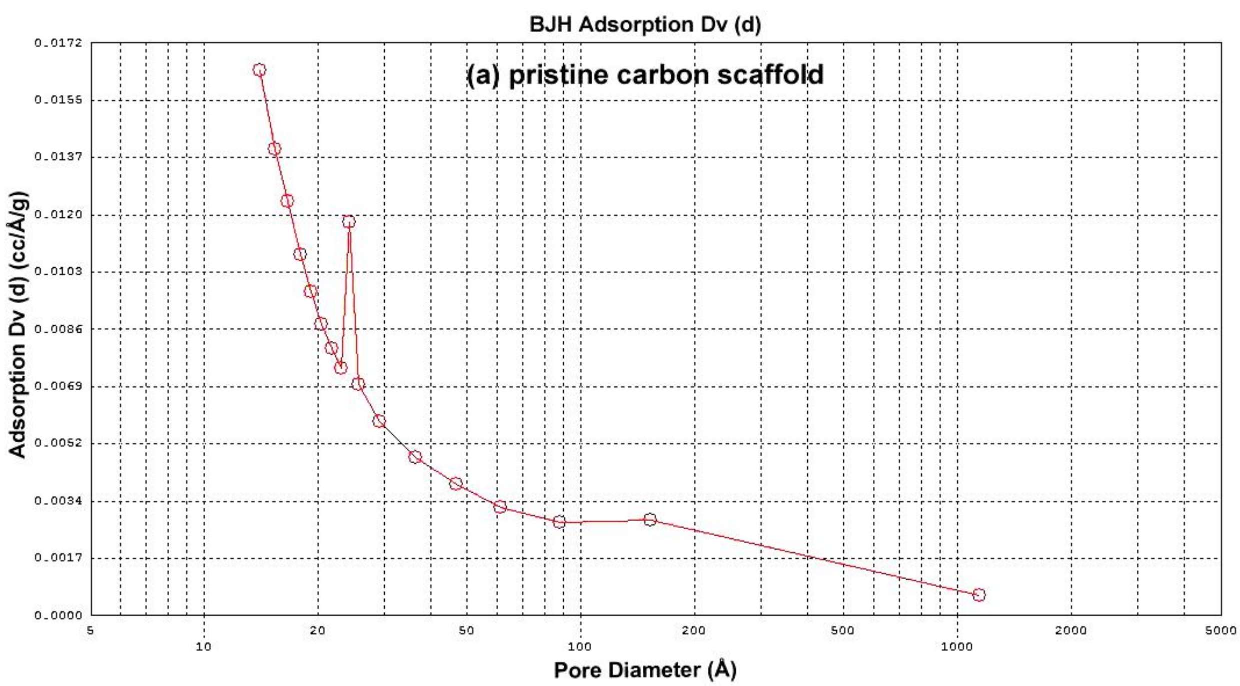


Figure S4a. Pore size distribution of pristine carbon scaffold.

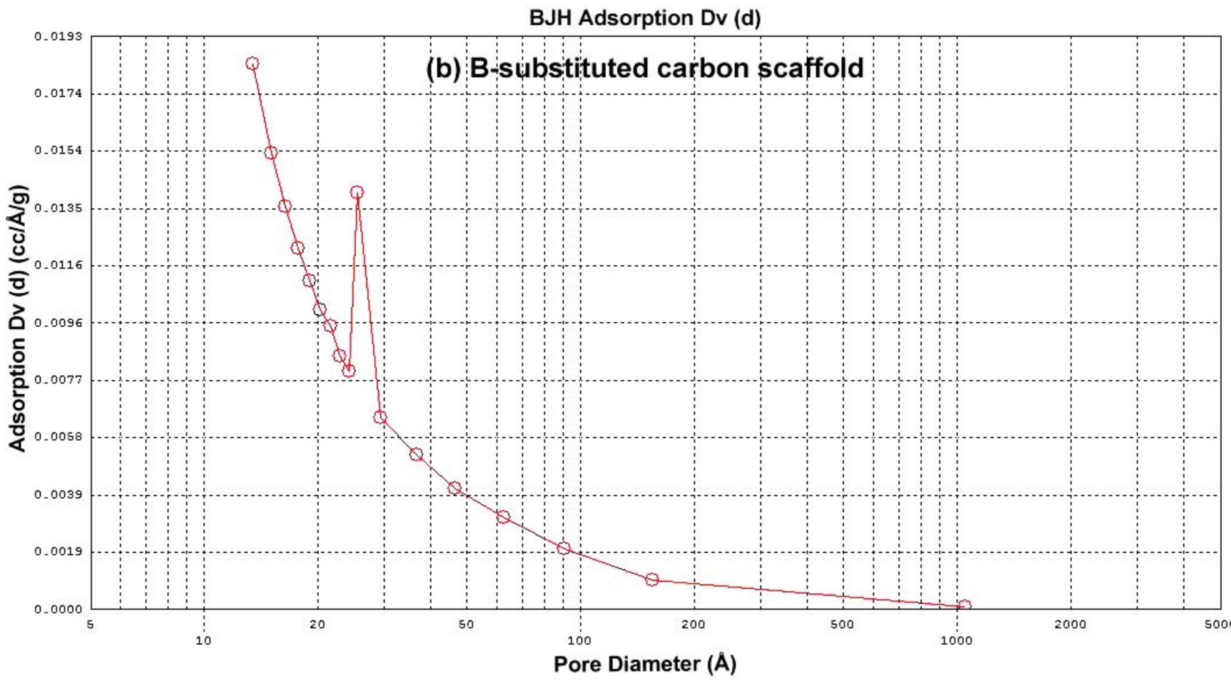


Figure S4b. Pore size distribution of boron-substituted carbon scaffold.

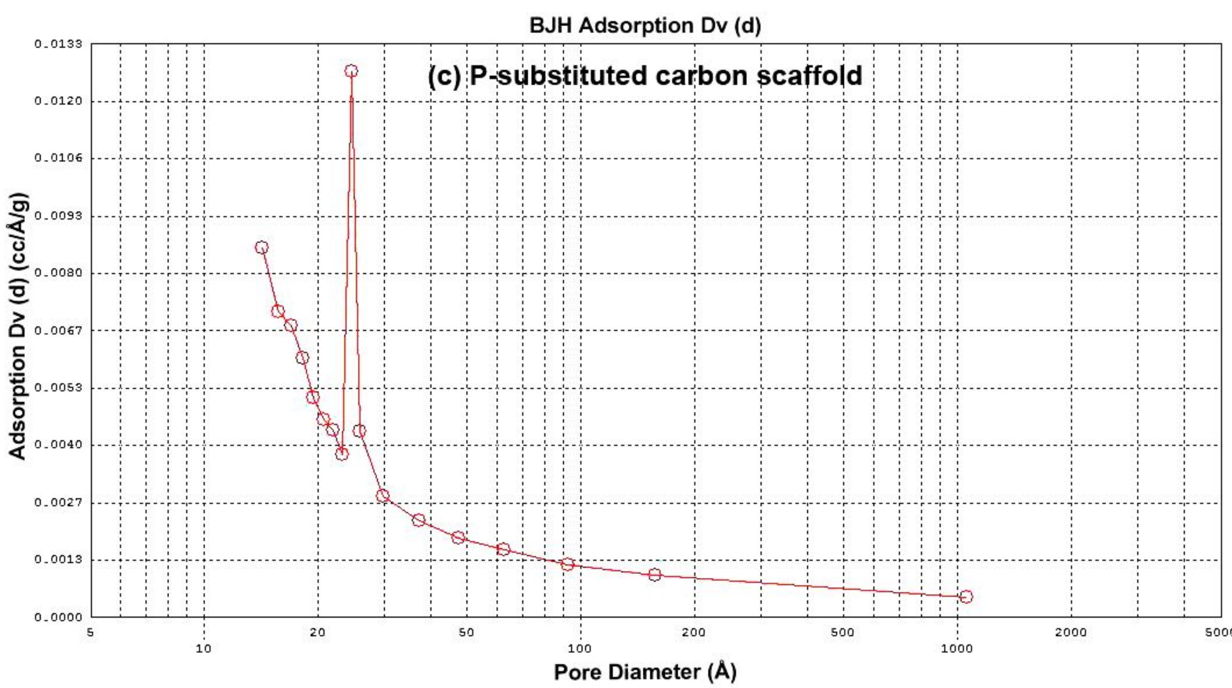


Figure S4c. Pore size distribution of phosphorous-substituted carbon scaffold.

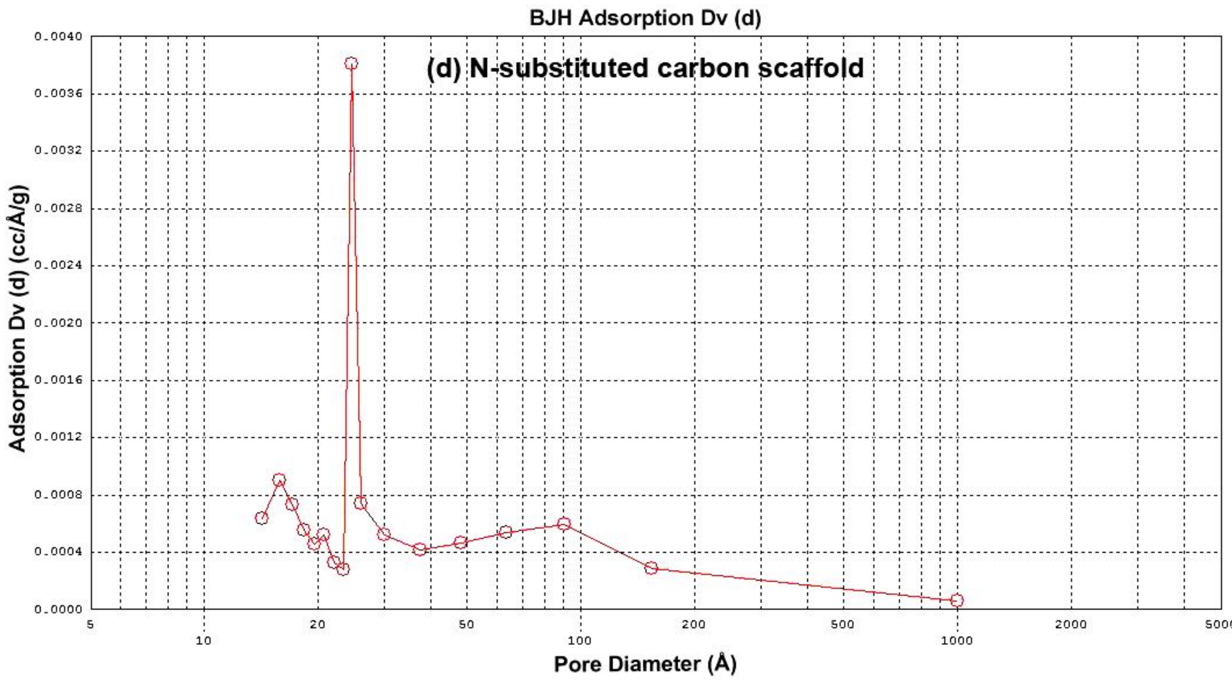


Figure S4d. Pore size distribution of nitrogen-substituted carbon scaffold.

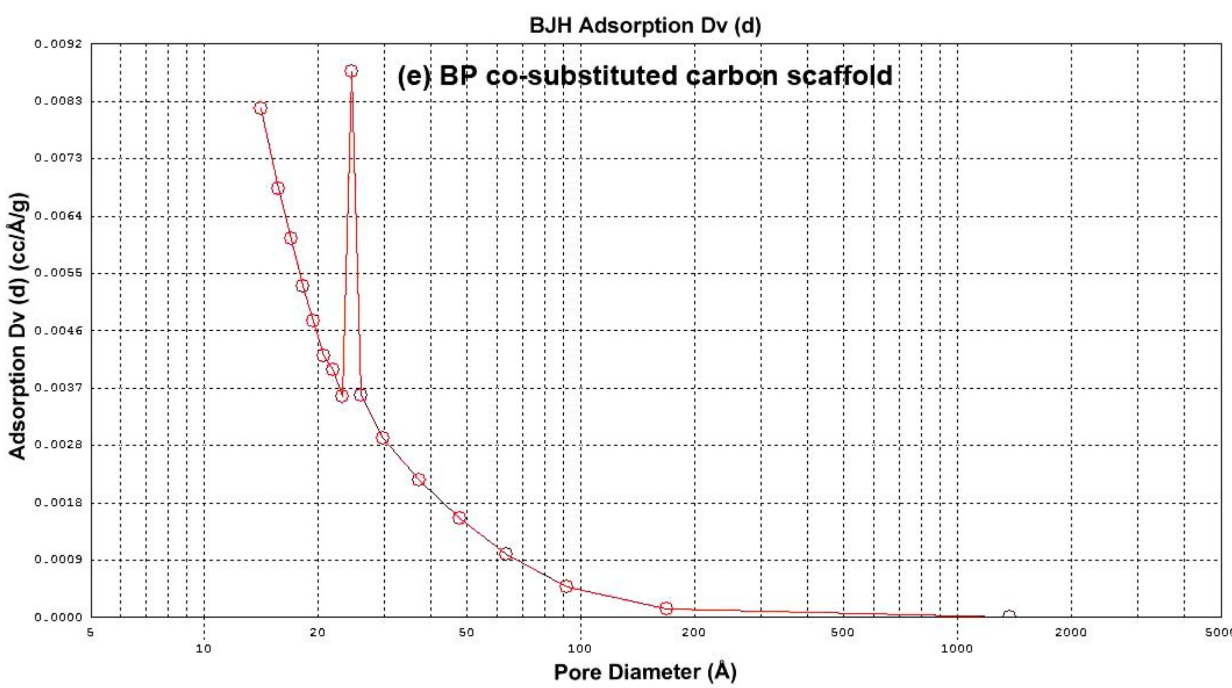


Figure S4e. Pore size distribution of boron/phosphorous co-substituted carbon scaffold.

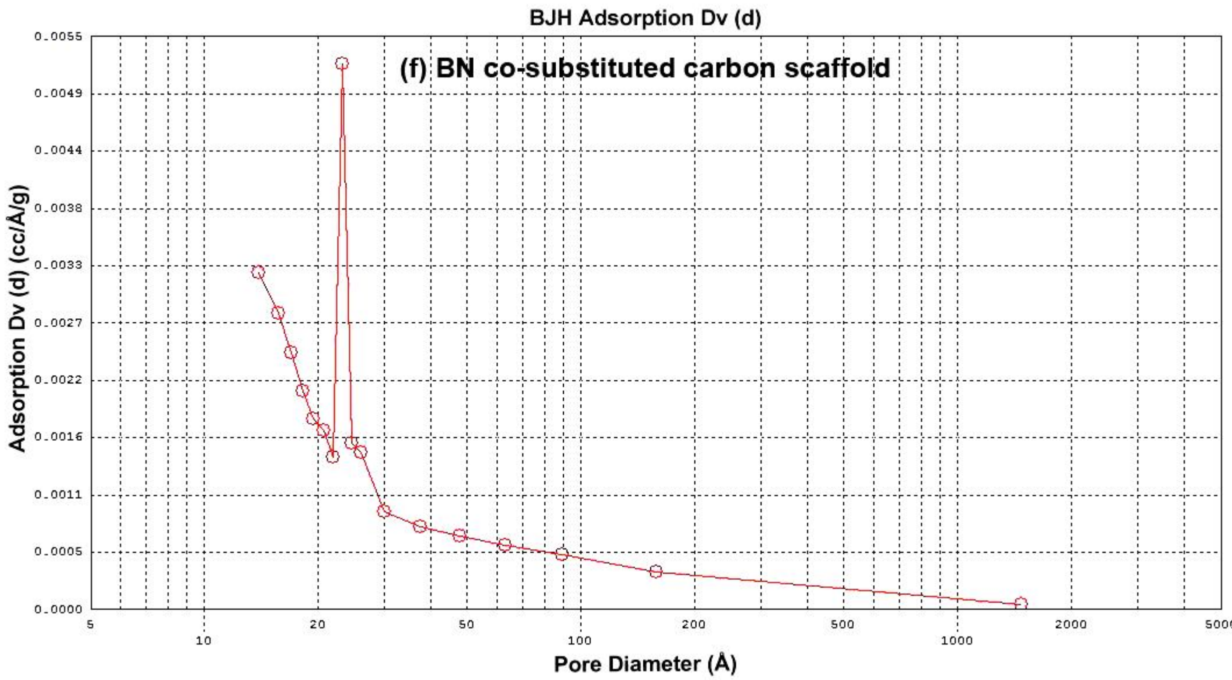


Figure S4f. Pore size distribution of boron/nitrogen co-substituted carbon scaffold.