

Structurally-controlled carbon materials with high pyridinic-nitrogen content

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Structural control of nitrogen-containing functional groups of carbon materials is essential for improving various applications such as catalysts and electrodes. However, most carbon materials contain various nitrogen-containing functional groups and the reasons for the high performance of various applications are unclear. It is because of the instability of functional groups upon heat treatment and unclear reaction pathway of carbonization reaction and also because of the unclear analyses of nitrogen-containing carbon materials by X-ray photoelectron spectroscopy. In order to improve these properties, it is necessary to introduce one type of functional group, but structural control of the nitrogen-containing carbon material has just begun in recent years. In this study, nitrogen-containing aromatic compounds with different nitrogen positions were carbonized at 973 K and structural control of pyridinic nitrogen was attempted.

This work compared 8 aromatic compounds with different nitrogen positions as precursors of carbon materials and discovered the precursor molecule, 1,7-phenanthroline, that forms carbon material with 92 % of pyridinic nitrogen at 973 K. The reasons for the high percentage of remaining pyridinic nitrogen were explained by molecular dynamic simulation with reactive force field and density functional theory calculation for reaction pathways of radical formation and simulated X-ray photoelectron and infrared spectra. The reasons for the formation of carbon materials with the high percentage of pyridinic nitrogen are mainly because of the low possibility to be hydrogenated on nitrogen atom in pyridinic nitrogen and high possibility of intramolecular scission of C-N bonding after hydrogenation of pyridinic nitrogen.