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Structural control and structural analysis of carbon materials

Abstract: Controlling structures of carbon materials is essential to attain superior properties for various applications. However, controlling structures in carbon materials is challenging because varieties of the reactions proceed during heat treatment to form carbonization and the structures of carbon materials are extremely complicated. Our group has synthesized carbon materials with an exceptionally high percentage of pyrrolic nitrogen at 873 K (94%), pyridinic nitrogen at 973 K (92%), tertiary nitrogen at 973 K (92–98%), pentagons at 773 K (96% retained from the precursor), pentagons-heptagons at 873–973 K (90%), edges with one sp²C–H on one benzene ring (SOLO) at 823 K (100%), and zigzag/armchair edges at 775 K (100% retained from the precursor) by the simple heating of the precursors in glass or quartz ampoules. Since catalysts were not used for the synthesis, mass production is possible and the carbon materials can be applied to many applications. In order to analyze the complicated structures of the carbon materials precisely, a combined analysis using X-ray photoelectron, Raman, and infrared spectroscopy, combustion elemental analysis, density functional theory calculation, and molecular dynamics simulations with a reactive force field was conducted. The origin of the ambiguous assignments of the spectral analyses of carbon materials was revealed.

Keywords: Carbon material, nitrogen, structural control, XPS, IR, Raman spectroscopy

Biography: Dr. Yamada received his Ph.D. from University at Buffalo, The State University of New York in 2008. He worked at National Institute of Advanced Industrial Science and Technology and Nippon Chemi-Con Corp. in 2009. He became an assistant professor in 2009 and an associate professor in 2019 at Chiba University in Japan.