No. 1401

Elucidation of Mechanism on Selective Adsorption of Br Ion by Nanocarbons

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Summary

Restricted molecules and ions in solid nanospace can play an important role in various phenomena such as catalytic reaction and energy storage. Consequently, elucidation of molecular structure and specific properties under nano-restricted condition is a kind of important research subjects. I have studied restricted structure of hydrated ion species confined in carbon nanospaces having different pore geometries and sizes. I could also find a specific adsorption phenomenon to selectively adsorb anions such as bromide ions into the micropore of carbon materials. Herein, I have investigated the adsorption mechanism of bromide ions into the carbon micropores using a kind of single-walled carbon nanotube (SWCNT) and two kinds of activated carbons (ACs) having different pore sizes.

SWCNT (d=1.2 nm) and ACs (w=0.63 nm (denoted as A7) and 1.03 nm (A20)) were selected as microporous carbons. RbBr was deposited into the micropores of carbon materials in aqueous solution. Both the pristine and the RbBr-adsorbed samples were characterized by adsorption isotherms (N_2@77 K), Raman, XPS, and XAFS spectra. Also, basic functional groups were quantitatively investigated by the titration method (Boehm method).

The results obtained strongly indicate that more Br ions can be adsorbed in the micropores of SWCNT and AC(A20), although small amounts of the ions can be restricted in the micropore of AC(A7) stemming from the size limitation of a hydrated Br ion into the narrower micropore. In addition, the pH values of the aqueous solution after the adsorption of Br ions were increased when more Br ions into the micropores, indicating that the protons can effectively initiate the co-adsorption of Br ions to neutralize excess-negative charge in the micropore. The results of XPS spectra strongly support such results because the band assigned to the bond between H^+ and Br^- can be observed for RbBr-deposited AC(A20). The results obtained in the present study can open new insights into the adsorption phenomena of anions to the microporous carbons.