Adsorption analysis of polymer and small molecules onto carbon materials based on adsorption isotherm measurements

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論 文 名：Adsorption analysis of polymer and small molecules onto carbon materials based on adsorption isotherm measurements（吸着等温線測定に基づく炭素材料へのポリマーおよび小分子の吸着挙動解析）

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論　文　内　容　の　要　旨

This thesis focusing on both a polymeric material like polybenzimidazole (PBI) and a small molecule like indole, primarily aims to provide insights into different aspects of adsorption onto carbon surfaces, contributing to the broader understanding and application in various fields. The surface modification of carbon materials is an effective method for enhancing the properties of carbon-based functional materials, especially via a polymer coating, which is advantageous owing to its intactness and simplicity. Moreover, the removal of uremic toxins such as indole using carbon-based adsorbents like mesoporous carbon (MC) is prominent for preventing the progression of chronic kidney disease (CKD). This research involves studying the adsorption kinetics, thermodynamics, and mechanisms involved in the interaction between these molecules and the carbon surface.

In chapter 2, The adsorption of PBI on various types of carbon black (Ketjen black; KB, Vulcan, Acetylene black; AB) with different surface morphologies and chemical compositions were analyzed via adsorption isotherm measurements. The adsorption behavior was compared to that of the PBI monomer unit, 1,3-bis(1H-benzo[d]imidazol-2-yl)benzene, and PBI was slower than that of the PBI unit, but PBI exhibited a larger adsorption capacity. PBI adsorption was driven by entropy, whereas the PBI unit adsorption was driven by enthalpy. The adsorption of PBI was more thermodynamically favorable on carbon surfaces with a higher crystallinity (lower oxygenation) owing to the easier detachment of solvent molecules from the carbon surface, leading to a higher adsorption constant.

In chapter 3, MC with a uniform diameter of 3.1 nm was used as an adsorbent for indole in aqueous media, and its thermodynamics were studied using the conventional adsorbent AST-120 as a control. Compared to AST-120, MC shows highly efficient indole adsorption as well as remarkable adsorption selectivity for indole in the presence of various amino acids. The excellent selectivity of MC can lower the dose of the adsorbent, which may improve the treatment strategy for CKD patients.

In chapter 4, adsorption kinetics of PBI and Indole over carbons have explored that the adsorption of PBI onto carbon materials is suitable for the efficient adsorption where the

trend of adsorption capacity, Γ_e and the adsorption rate constant, k_2 was KB > Vulcan > AB. The adsorption of indole on MC is faster than that on AST-120, suggesting the particle size and pore structure of MC may play a vital role in determining the adsorption rate. The intraparticle diffusion is a rate- controlling step on both PBI and Indole adsorption together with the adsorption reaction.

In conclusion (chapter 5), provide a concise summary of results alongside a thoughtful exploration of future perspectives which can effectively communicate the significance of the research outcomes and inspire further scientific inquiry in the field of adsorption and carbon material applications.