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Interaction mechanisms of Ionizable Organic Pollutants with Aromatized Biochar: Adsorption Experiments and DFT Calculations

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The molecular interaction between biochars and ionizable organic pollutants (IOPs) are of great concern in natural environments, however the underlying mechanisms and their quantification under different pH range are not vivid. The adsorption of IOPs onto high temperature biochars derived from bamboo wood biomass (BW700) was conducted to quantify the various interactions between sorbent surface and IOPs under different pH conditions. The aromatized surface of BW700 were characterized by Fourier Transformed Infrared spectroscopy (FT-IR), Brunauer-Emmet-Teller (BET) specific surface area with N2 and CHN elemental compositions. Seven IOPs were selected as model sorbates, and batch sorption experiments were conducted to quantify the ratio of π-π interactions and hydrogen bonding interactions. The pH-dependent adsorption curves and the adsorption isotherms not only indicated that the adsorption capacity was related with species of IOPs, but also showed the presence of adsorbing peak owing some of the other mechanisms when taking the ice-like adlayer into consideration. Finally, density functional theory (DFT) calculations provided a possible structure of the complex combined with ice-like adlayer with aromatic substrate of BW700, and indicated that the formation of extra adsorption sites originated from the X–H ... O–H ... π interactions. The contribution of π-π interactions, hydrogen bonding interactions and X–H ... O–H ... π interactions were distinguished by the pKa value of IOPs owing to their species. Our findings provide new insight for distinction and quantification of various interactions under different pH conditions, and it is the first time to put forward the X–H ... O–H ... π interactions for the interaction mechanism of IOPs with biochar.