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Variation of chemical reactions of organic molecules on the Si(5 5 12) surface

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In the present study, we present our first-principles and STM investigations on the adsorption structures of benzene, pyridine, and aniline on the high-index Si(5 5 12)2x1. These structures are different from those observed on low-index Si surfaces: benzene molecules exclusively bind to two adatoms, i.e., with di-σ bonds between carbon atoms and silicon adatoms, leading to the loss of benzene aromacity; in contrast, pyridine molecules interact with adatom(s) either through Si-N dative bonding or di-σ bonds. Dative bonding configurations with pyridine aromacity are more stable than di-σ bonding configurations.

Thus, the dative bonding of nitrogen-containing heteroaromatic molecules provides a strategy for the controlled attachment of aromatic molecules to high-index surfaces. On the other hand, aniline is adsorbed dissociatively on the surface.