

Abstract Submitted
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Benzene Derivatives Adsorbed to the Ag(111) Surface: A Binding Site Study DANIEL MILLER, SCOTT SIMPSON, NINA TYMINSKA, EVA ZUREK, University at Buffalo, ZUREK GROUP TEAM — Dispersion corrected Density Functional Theory (DFT) calculations were employed to study the interaction of benzenes mono and disubstituted with functional groups encompassing a region of the activated/deactivated spectrum. Benzenes substituted with weak activating or deactivating groups like methyl and fluoro, respectively, do not have a strong site preference for adsorption to the Ag(111) surface. Strong activating (N(CH₃)₂) and deactivating (NO₂) groups, on the other hand, have a distinct site preference. The nitrogen in the former prefers to lie above a silver atom (top site), but in the latter an Hhcp site of the Ag(111) surface is favored. Benzenes derivatized with classic activating groups donate electron density from the highest occupied molecular orbital (HOMO) of the molecule to the surface, and those functionalized with deactivating groups withdraw electron density from the surface into orbitals that are unoccupied in the gas phase. In the case of disubstituted benzenes, the strong activating/deactivating groups control the site preference and other groups assume sites that are, to a large degree, dictated by their positions on the benzene ring. Surface adsorption alters the relative stabilities of the ortho, meta and para positional isomers of disubstituted benzenes.

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