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Forces and Dynamics in Aromatic Overlayers on Metal Surfaces[1]

SHAFAT MUBIN, KRISTEN FICHTHORN, Pennsylvania State University — Organic thin films have been the subject of intense research because of their suitability for applications in molecular electronics. The beneficial properties of these films are sensitive to the structure of the film. However, predicting and controlling organic thin-film structures is still a significant challenge. Owing to computational requirements, first-principles calculations cannot probe the link between thin-film deposition conditions and film structure. In this talk, we will discuss a multi-scale approach applied to quantify structures and dynamics of a thin film of benzene on Ag(111). Based on first-principles calculations, we developed a force field to describe the interaction of benzene with Ag(111). We applied this force-field to describe several aspects of this system, including its order-disorder phase transition and its desorption kinetics. Despite the apparent simplicity of this vdW dominated system, it exhibits surprising complexity in binding site preference and in ordering, leading to an interesting interplay between pi-conjugated electrons of benzene and surface-state electrons of Ag(111).

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