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Bonding of anthracene derivatives to a Cu (111) surface: a combined STM and DFT study JONATHAN WYRICK, YEMING ZHU, DANIEL SALIB, CONNOR HOLZKE, University of California at Riverside, ZHIHAI CHENG[1], The National Center for Nanoscience and Technology, China, LUDWIG BARTELS, University of California at Riverside — We compare and contrast three anthracene derivatives whose 9,10 hydrogens are replaced by the elements O, S, and Se respectively that act as "feet" binding the molecules to a Cu (111) substrate. DFT calculations are compared with and shed light on STM data for the three molecules. We analyze the three species in terms of their geometric and electronic structure upon adsorption, taking into account the competing effects that the "feet" have with the anthracene moiety in their interactions with the underlying Cu surface.

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