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Effect of Substrate Chemistry on the Adsorption of Olympicene Radical: A vdW inclusive DFT study[1] JERONIMO KARA, University of Central Florida, HANDAN YILDIRIM, Purdue University, ABDELKADER KARA, University of Central Florida — We investigate the effects of surface chemistry on the adsorption characteristics of the Olympicene radical on Au and Pt(111) surfaces using vdW inclusive density functional theory (DFT) employing the optimized vdW-DF and vdW-DF2 methods. Adsorption characteristics such as adsorption energy, adsorption geometry, electronic structure, charge transfer, and charge redistribution will be presented. The effect of substrate electronic structure on the nature of bonding will be discussed. Comparison on the nature of bonding will be presented with our previously reported results on the adsorption of Olympicene radical on Cu(111) to provide a more complete picture.

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