

Abstract Submitted
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Trends in Adsorption Characteristics of Organic Molecules on Transition Metal Surfaces: Role of Surface Chemistry and van der Waals Interactions¹ HANDAN YILDIRIM, School of Chemical Engineering, Purdue University, ABDELKADER KARA, Department of Physics, University of Central Florida — The accurate description of interface characteristics between organic molecules and metal surfaces has long been debated in theoretical studies. A well-founded description of interface geometry and adsorption energy is highly desirable for these systems. Using first principles calculations with the inclusion of van der Waals interactions, we examine the adsorption characteristics of a few organic molecules on several transition metal surfaces. Our aim is to obtain insights into the role of vdW interactions in the adsorption characteristics as well as to build an understanding on how these functionals treat the adsorption on varying surface chemistries. Furthermore, the comparisons made between the results obtained using different vdW functionals for each organic molecule type provide the means to assess their performance.

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