

Abstract Submitted
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First Principles Investigation of the C3 Coefficients for Molecular Adsorption on Transition Metal Surfaces¹ ABDELKADER KARA, JERONIMO MATOS, University of Central Florida, HANDAN YILDIRIM, Purdue University — C6 coefficients are used to investigate the strength of the long-range interactions for weakly interacting dimers as a function of separation distance. These coefficients are useful both as a measure for the accuracy of the various van der Waals (vdW) inclusive methods as well as reference for use in large-scale molecular dynamics simulations. In the case of molecule-surface interaction, the C3 coefficient is the counterpart to the C6 coefficient that is used for testing the interaction of dimers. We will present the results of the vdW inclusive density functional theory (DFT) calculations evaluating the C3 coefficients for the adsorption of M/X(110) and X(111), with X: Ag, Au, Cu, Pt, Pd, Ni, Rh and M: Benzene, Thiophene, Sexithiophene, Pentacene and Olympicene, as described by the PBE exchange-correlation functional and the self-consistent vdW-DF, optimized vdW-DFs and vdW-DF2 functionals.

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abdelkader kara
University of Central Florida

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