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Adsorption of 2-thiophene curcuminoid molecules on a Au(111) surface

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Abstract. We provide a systematic ab-initio study on the adsorption of 2-thiophene curcuminoid (2-thphCCM) molecules on a Au(111) surface. In this work we present the determination of the optimal configuration of a single molecule on the surface as well as a detailed study of the energetics of the different arrangements of two molecules considering their intermolecular interactions. We simulate the STM measurements associated with the optimal configuration and compare it with the experimental data.

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Keywords: thiophene molecules, self assembled monolayers, STM.

1. Introduction

The physical properties and hence the potential applications of nano-devices can be modified dramatically by exploiting its interplay with suitable designed and synthesized molecules [1, 2, 3, 4]. This idea has grown into a leading research theme, namely molecular electronics, that involves extensive collaboration between different disciplines such as organic chemistry, material sciences and condensed matter physics [5, 6, 7, 8]. Recently, self-assembled monolayers (SAMs) have received wide attention both from experimental measurements and theoretical calculations [9, 10, 11]. Special interest has been devoted to thiolates derivatives molecules and thiophenes over gold surfaces [9, 12, 13, 14, 15]. This interest stems from potential applications in areas ranging from lubrication control to electronic applications [16].

Proper understanding of the binding mechanisms in the interaction between noble metals and organic molecules is of the utmost importance in molecular electronics,