

Preface

Over the last 10 years the world has been involved in a technological revolution. Every day newer and smaller devices, essential to life, appear on the market: mobile phones, computers, laptops, netbooks and so on. Nowadays, it is possible to have a portable device with 1 Terabyte capacity compared to the 2 Gigabytes being the maximum 4 years ago. This is just an example of how rapid the development in technology can be. The main aim is to decrease the dimensions while increasing the efficiency and capability of the product. In nanotechnology, one is particularly interested in manipulating and designing objects at a nanoscale to be implemented in everyday products. The main aim is to decrease the dimensions while increasing the efficiency and capability of the product. In nanotechnology, one is particularly interested in manipulating and designing objects at a nanoscale to be implemented in everyday products. The organic/inorganic interfaces are excellent candidates for building electronic devices at a nanoscale, as well as optical sensors.

Developments in nanotechnology are related to the investigation of scanning probe microscopy (SPM), allowing analysis to be done at the nanoscale (10^{-9} m). With STM they made possible the visualization of surfaces and interfaces by employing the principles of quantum mechanical tunneling. The atomic force microscope (AFM) by using the forces acting between the surface and the tip, an image of the surface or an interface can be obtained. These new techniques make possible an understanding of the physical structure and properties at the nanoscale, changing the focus from the top-down to the bottom-up strategy of building nanodevices.

Experimental methods based on SPM can give invaluable information concerning the templates and the molecular aggregations. However, in many cases atomic or even molecular resolution is not possible, and different theoretical methods will therefore play an important role in resolving the image and modeling the supramolecular templates.

The aim of this thesis is to present a theoretical study of self-assembly of flat organic molecules (such as melamine, PTCDA, PTCDI, NTCDA, NTCDI and DNA derivative molecules) on the Au(111) metal surfac. In order to describe in

detail the assembly of the molecules, a systematic approach to building molecular superstructures based on the notion of binding sites has been proposed. First, one must identify all possible sites for hydrogen bonding between molecules. Then how to form molecular pairs and larger structures using all possible combinations of these binding sites has been considered. In this way, all possible dimers, chains and 2D monolayers of melamine, dimers and chains of PTCDA and PTCDI molecules have been considered. The energies of these structures are calculated using the density-functional theory SIESTA code. The strength of hydrogen bonding in various molecular arrangements is analysed. The theoretically predicted monolayer structures are in very good agreement with the results of STM measurements.

<http://www.springer.com/978-3-642-30324-1>

Self-Assembly of Flat Organic Molecules on Metal
Surfaces

A Theoretical Characterisation

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2012, XVI, 169 p., Hardcover

ISBN: 978-3-642-30324-1