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Contents

Chapter 1

A study on adsorbed RuTPP/Cu(110) and CO-RuTPP/Cu(110) structure

1.1 Geometry of adsorbed considered

1.1.1 Geometry structure of isolated RuTPP/Cu(110)

Starting from a relaxed isolated gas phase molecule laid over the surface in a short bridge configuration as shown in figure (citare la figura), and putting the parameters shown in appendix (appendice), the relaxing was carried out. The interaction of RuTPP with Cu(110) has brought some changing of the position of the four macrocycles and a rotation of the phenyl rings (citare le tabelle). The moving and rotation of the vector distance between the the center of mass for each phenyl ring and the metal core (Phr-Ru) and the rotation of the normal vector of the plane of any ring were considered to quantify the dynamics of them. For (Phr-Ru) module was not observed particular changing, instead an evident changing of the angle between (Phr-Ru) and the z cartesian versor γ was observed showing a rotation of about 10 degrees. Further rotations have been observed even for the planes of the rings, rotating the plane vectors of about 20 degrees respect the gas phase configuration. In addition to was considered even the the shortest distance between the metal core and the copper surface, resulting of 2.563 Å. The structure show for the view (citare la vista) even a bending due a conformation of the phenyl rings. The desorption energy of RuTPP on Cu(110) was calculated using the rela-

Macrocycle	distance	α (1,0,0)	β (0,1,0)	γ (0,0,1)
		RuTPP		
left ring	6.26	0.0	90.	90.
right ring	6.34	0.0	90.	90.
upper ring	6.34	90.	0.	90.
bottom ring	6.33	90.	0.5	89.
		Isolated-RuTPP/Cu(110)		
left ring	6.36	5.	0.	81.
right ring	6.36	5.	0.5	80.
upper ring	6.36	5.	1.	80.
bottom ring	6.36	5.	0.5	81.
		RuTPP/Cu(110)		
left ring	6.07	18.	86.	72.
right ring	6.06	18.	86.	72.
upper ring	6.42	89.	10.	80.
bottom ring	6.40	89.	11.	79.

Table 1.1: Distances between the Ruthenium atom and centre of mass of the different phenyl rings, and angles between the distance vector and the Cartesian coordinate directions, with α, β and γ the angles between the vector considered and the coordinates x, y and z rispectively, as indicated for the isolated RuTPP molecule and adsorbed on Cu(110).

tion (scriverla) and it has resulted of ..... Finally has been possible a comparation between the STM images carried out in laboratory and those calculated using (citare la teoria) for 0.5 eV and 1 eV. The images obtained are in good agreement (commentare la luminosita se è possibile). (inserire figure STM 2sperimentali e2 teoriche e geometria 3).

1.1.2 Geometry structure of RuTPP/Cu(110) ((2,-6);(4,-2))

The configurations ((2,-6),(4-2)) and (citare l'altra in forma matriciale entrabmi) examined in laboratory were simulated using the same procedure explained in the section before. The first structure considered has shown a weak contraction of the (Ru-Ph) rings for the right and left rings shown in the figure (mettere l'orientamento della figura). Furthermore of the evident rotations were observed for (Ru-Ph), about of 18 degrees for γ and α degrees, in the left and right ring

Macrocycle	γ (0,0,1)
RuTPP	
upper ring	20.
right ring	21.5
bottom ring	21
left ring	22.
Isolated-RuTPP/Cu(110)	
upper ring	47.
right ring	44.
bottom ring	45.
left ring	43.
RuTPP/Cu(110)	
upper ring	38
right ring	2.
bottom ring	39
left ring	8.

Table 1.2: The angles between the normal vector of the phenyl rings plane and the z coordinate.

(specificare sempre l'orientamento) while for the upper and the bottom rings about 10 degrees for β and γ angles. The angles resulting for the ring plane vectors were risultated almost perpendicular at the z axis for the right and left rings precisely 2 and 8 degrees, and a rotation of about 20 degrees were resulted for the upper and lower rings.