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Electronic and reactivity properties of phthalocvanines have Iron been investigated using Density Functional Theory and scanning tunneling microscopy, Phthalocyanines (Pcs) are organic molecules possessing a central cavity which can accommodate a single metal atom (M). Metal phthalocyanines (MPcs) are able to adsorb on a variety of with ordered supports. structures determined by molecule-molecule and molecule-substrate interactions. Employing metal phthalocyanine selfassembling properties, it is possible to obtain model systems for biomimetic 1-D centers. where active unexpected properties may stem from the utmost low dimensionality. In our work we focus on Iron phthalocyanines deposited on ultrathin alumina films. These molecules self-assemble in highly ordered structures, stable enough to provide optimal candidates for model single atom catalysis. We found that it is possible to control the FePc's selfassembly decorating the alumina laver with Cu nanoclusters, switching between adsorbed structures governed by or molecule-molecule or molecule-substrate interaction

Self-assembled monolayer films of Iron phthalocyanines on thin alumina films: characterization and properties

Figures

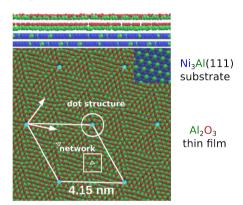


Figure 1: (Structural model of Al₂O₃/Ni₃Al(111))

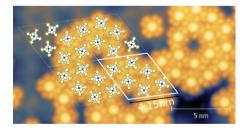


Figure 2: (STM image of FePcs on $AI_2O_3/Ni_3AI(111),$ together with DFT model)

nanoPT2018 Lisboa (Portugal)