

Self-assembly of flat organic molecules on metal surfaces : a theoretical characterisation

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Abstrak

Manuela Mura's thesis is devoted to ab initio studies of self-assembled organic molecules on a gold surface. This area of research is particularly vibrant because of the various applications such studies have in nanoscience and surface chemistry and physics. In this thesis Manuela Mura uses theory to suggest atomistic models for the observed assembled and she proposes an assembly mechanism. The methods and results developed as part of this work will be of wide interest to physicists and chemists working on the assemblies of organic molecules on crystal surfaces.