Self-assembly of NC-PH_3-CN molecules on Ag(111): Formation of 2D hydrogen-bonded and organometallic networks

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Abstract

Ditopic linear cyano-organic molecules are of great interest for the generation of bidimensional networks on metallic surfaces, because of their ability to form self-assembled hydrogen-bonded all-organic monolayers, as well as shape-resistant organometallic networks upon addition of transition metal atoms, to which cyano groups are known to bind strongly.

In this poster we show a study for the case of the NC-Ph_3-CN molecule on a Ag(111) surface, before and after addition of cobalt atoms. In the case of the all-organic monolayer, different structures are proposed (see Figure 1), and their relative stability is discussed. We also discuss the effect of the surface upon the intrinsic binding scheme of the cyanophenyls, modelled by a planarization of the structures. For the Co-coordinated networks, an energetic explanation is found for the experimental 3-fold coordination of the cobalt centers, comparing it with an alternate 4-fold coordination (see Figure 2).

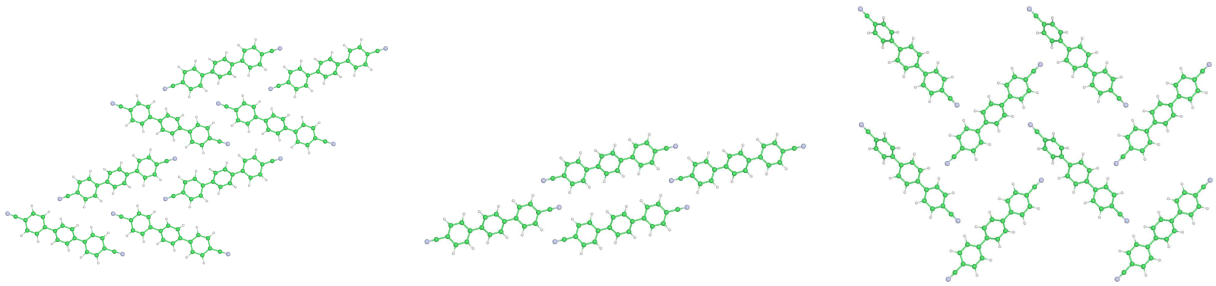
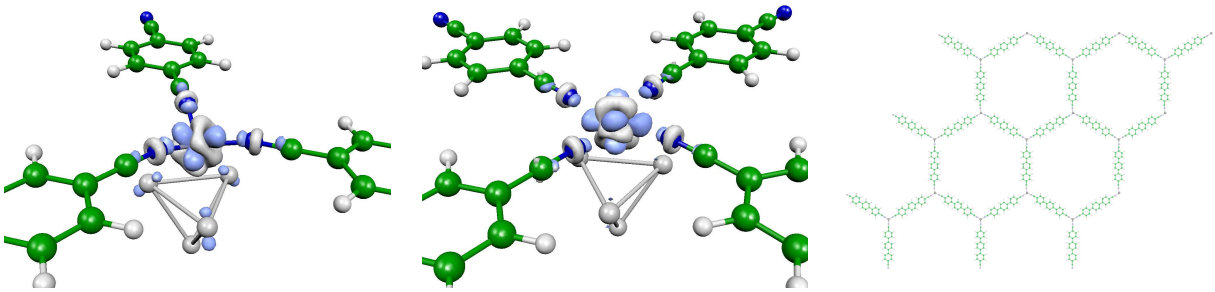


Figure 1: Three different patterns proposed for NC-Ph_3-CN self assembly.



3-fold coordination 4-fold coordination Honeycomb periodic structure

Figure 2: Induced charge density plots around the cobalt atom for 3-fold and 4-fold coordination. The corresponding honeycomb lattice for the 3-fold coordination is also shown.