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Theoretical Modelling of Self-Assembly of Molecular Networks
MANUELA MURA, NATALIA MARTSINOVICH, LEV KANTOROVICH, King's College — The phenomenon of self-assembly of atomic and molecular superstructures on crystal surfaces has attracted an increasing interest in nanotechnology. Self-organised nano-templates where the self-assembled monolayer traps other molecules with selected functional properties, can be used as building blocks for larger nanoscale structures. These superstructures can form chiral domains ranging from 1D chains to 2D monolayers. In particular, there have been many scanning tunneling microscopy (STM)studies of self-assembly of melamine, perylene tetra-carboxylic di-imide(PTCDI) or perylene tetra-carboxylic di-anhydride (PTCDA) molecules on the Au(111). STM images of these networks do not reveal the exact details of the intermolecular bonding and process of network growth. It is therefore the task of theory to determine the exact atomic structure of these networks. We present a theoretical study of self-assembly of molecular networks based on different molecules by using a systematic approach to build molecular superstructures. The energies of these structures are calculated using the density-functional theory SIESTA code. The theoretically predicted monolayer structures are in very good agreement with the results of STM measurements.

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