

SELF-ASSEMBLY OF POLYCARBOXYLIC ACIDS INTO TWO-DIMENSIONAL MOLECULAR NETWORKS: A THEORETICAL STUDY

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The phenomenon of self-assembly of molecular superstructures is attracting an increasing interest in nanotechnology due to possible applications in materials science and molecular electronics [1]. Self-assembly of molecules is controlled by specific intermolecular interactions. In particular, hydrogen bonds (H-bonds) are among the strongest intermolecular interactions, they are directional and give rise to complex supramolecular networks on a variety of substrates [1-4].

This abstract presents our theoretical studies of self-assembly of benzenedicarboxylic acids into hydrogen-bonded supramolecular structures. Experimental scanning tunnelling microscopy studies of self-assembly of these molecules [4] revealed the network structures based on closely packed H-bonded chains of molecules. Here we model the process of aggregation of isolated molecules into ordered two-dimensional (2D) networks, using a combination of force field molecular dynamics and Monte Carlo calculations, with the aim to investigate the emergence and evolution of ordered supramolecular structures.

Our results show the initial rapid formation of short H-bonded molecular chains, which, in some conditions, may then assemble parallel to each other into 2D sheets due to van der Waals interactions between the chains. We find that a high density of molecules leads to compact and highly ordered structures consisting of close-packed molecular chains, similar to the experimental images [4], whereas a low concentration of molecules leads to long chains which do not assemble into compact 2D structures.

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