Self-assembly of organic molecules onto surfaces: computer simulations

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Abstract

The prediction of supramolecular self-assembly onto solid surfaces is still challenging in many situations of interest for nanoscience. In particular, no previous simulation approach has been capable to simulate large self-assembly patterns of organic molecules over reconstructed surfaces (which have periodicities over large distances) due to the large number of surface atoms and adsorbing molecules involved. We show here how a novel simulation technique (Self-Assembly of Nano Objects, SANO) is able to perform atomistic simulations of hundreds of organic molecules over large surfaces (50x50 nm^2) self-assembling in thermodynamic equilibrium. The technique is illustrated with several examples. We consider (a) [1] the self-assembly patterns of di-indenoperylene (DIP) molecules over different reconstructions of the Au(111) surface [1] and (b) tri-adamantyl (TAB) benzene molecules onto Ag(111) [2]. In both cases, we compare with experimental STM images.

The simulation strategy opens interesting perspectives to tune the supramolecular structure by simulation design and surface engineering if choosing the right molecular building blocks and stabilising the chosen reconstruction pattern.

References

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