Shobhana NARASIMHAN
Theoretical Sciences Unit and School of Advanced Materials Jawaharlal Nehru Centre for Advanced Scientific ResearchBangalore, India

Descriptors from Small Data: Simple Yet Successful Descriptors for Self Assembly of Organic Molecules on Surfaces

Abstract:

Self-assembly is probably the most promising route to constructing devices at the nanoscale. The challenge is to predict the geometries of self-assembled architectures by utilizing only the properties of the individual molecular components. Working jointly with experimentalists, we have explored the feasibility of such an approach for a model set consisting of three host molecules (carboxylic acid derivatives of phenyleneethynylene) and five guest molecules (napthalene, phenanthrene, benzo-c-phenanthrene, benzo-ghi-perylene and coronene), self-assembled on graphene.

Using insights gained from scanning tunneling microscopy experiments and density functional theory calculations, we have formulated simple descriptors that can successfully predict the geometries of the host-guest architectures self-assembled from our palette of organic molecules. A structure map can be constructed using host and guest descriptors, with structures of the same type clustering in descriptor space. Though these descriptors can be evaluated at essentially zero computational cost, they correctly reproduce experimental observations, including the structural transitions exhibited by host assemblies upon introducing certain guest molecules. The descriptors are validated by their success in predicting not just the ground state geometry but also the energetic difference between competing structures for molecules that did not form part of of the training set used when formulating the descriptors.

This work suggests a novel approach toward the rational design of self-assembled nanostructures. It was performed in collaboration with Sukanya Ghosh at JNCASR, and Pratap Zalake and K. George Thomas at IISER Thiruvananthapuram.