Mathematical Tools for Molecular Self-Assembly

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The equilibrium state of a molecular self-assembly process is notoriously difficult to predict *via* conventional computational methods. Thermodynamics requires that the self-assembly process minimizes energy and also maximizes entropy; the former favors the assembly of molecules into larger structures, whereas the latter favors the random dispersion of molecules across the substrate. This presentation will introduce a realistic model for the molecular self-assembly process, as well as the *equivalence class sampling* (ECS) technique for computing the equilibrium properties of this model. By cleverly compressing the amount of information contained in the model, the ECS technique incorporates both entropy and energy (as opposed to energy alone) into the computational framework. As a consequence, the ECS technique is able to efficiently predict the kinds of structures that occur at equilibrium in the self-assembly process. Example calculations for the self-assembly of graphene precursors on Cu(111) surfaces will be presented, and remaining challenges will be discussed.

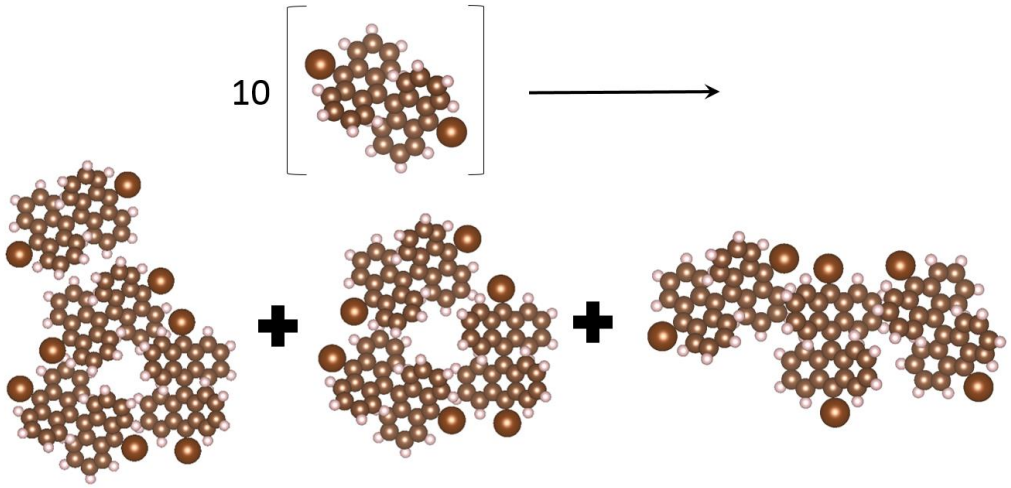

Figure: Prediction of the structures formed by self-assembly ten bianthryl-dibromo molecules on a Cu(111) surface at low temperature. The Cu(111) surface (not explicitly shown) is in-plane with the page. The ECS technique predicts the combination of structures that appear from the self-assembly process.