Semiconducting organic thin films are interesting as potential materials for large area, mechanically flexible electronic displays. Among the small conjugated molecules suggested for organic electronic applications, pentacene is particularly important for its relatively high field effect mobility. While considerable progress has been made towards fabricating organic electronic displays, there is still much to be learned about the link between structure and molecular packing of pentacene thin films and the growth mechanisms that produce these structures.

We have undertaken multi-lengthscale simulations to understand how the performance of organic thin films is affected by the choice of organic compound, substrate surface, and deposition conditions. The chemical bonding interactions of the pentacene molecule on the Si (100)-(2x1) surface is investigated using a combination of tight-binding simulations and \textit{ab initio} Gaussian™ calculations. A fairly comprehensive set of adsorption energies allows the determination of preferred configurations which confirm the strong monolayer adsorption observed in experimental STM images. Binding energies are computed, using Gaussian, for the weaker intramolecular van der Waals interactions between pairs of pentacene molecules as a function of orientation and interaction with various substrates, including passivation with either cyclopentene molecules or silicon dioxide. These binding energies are used as the input to a mesoscopic scale study of the layer-by-layer deposition of organic thin films in lattice-based Kinetic Monte Carlo simulations, providing a rich and varied morphology diagram.