

Multiscale modelling for the prediction of two dimensional molecular self-assemblies on a passivated Si surface

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The self-assembly of two-dimensional (2D) molecular structures on a solid surface relies on the subtle balance between non covalent intermolecular and molecule-surface forces. The energetics of 2D molecular lattices forming different patterns on a passivated semiconductor surface are here investigated by means of multi-scale atomistic simulations. Density-functional theory and metadynamics firstly provide a best guess for the lowest-energy adsorption sites of single molecules and dimers. Subsequently, molecular dynamics simulations of extended molecular assemblies with empirical forces, yield the most favorable lattice structures at finite temperature and pressure. Comparison between theoretical and experimental results, obtained by scanning tunneling microscopy (STM) on molecular monolayers adsorbed on silicon under ultra-high vacuum at low temperature, allows to appreciate the relative strength of the dispersion forces between molecules and the silicon surface, as well as greatly helping in the analysis of STM images, thereby demonstrating the interest of such a predictive approach for supramolecular chemistry on semiconductor surfaces.