Molecular assembly

Ma. Watkins, UCL

Properties of adsorbed molecules and defects
Simulation – AFM, STM

Statistics of defects in amorphous materials

Complex interfaces – alignment critical – hybrid functionals

In solution too!

MM Region (Vacuum)

QM Region (Surface + Molecule)

MM Region (Bulk)

Excited states & vibrational spectroscopy

Molecular assembly

Excited states & vibrational spectroscopy

Properites of defects and adsorbed molecules

SPM simulation – AFM, STM