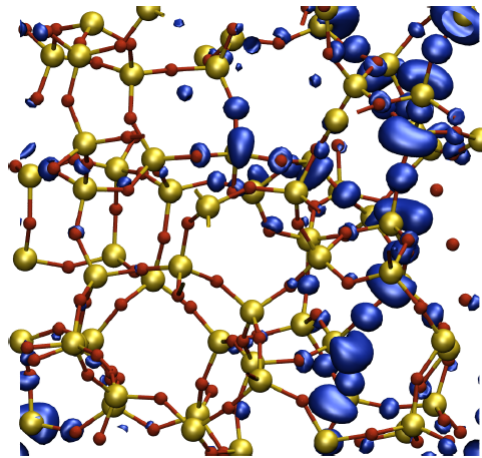
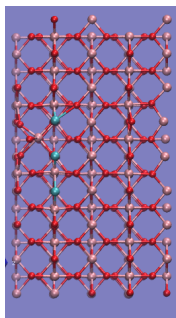
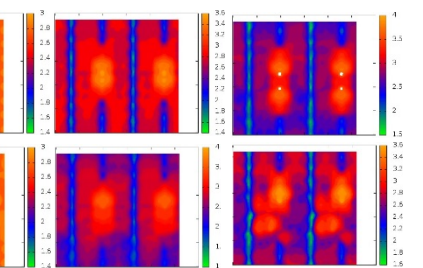
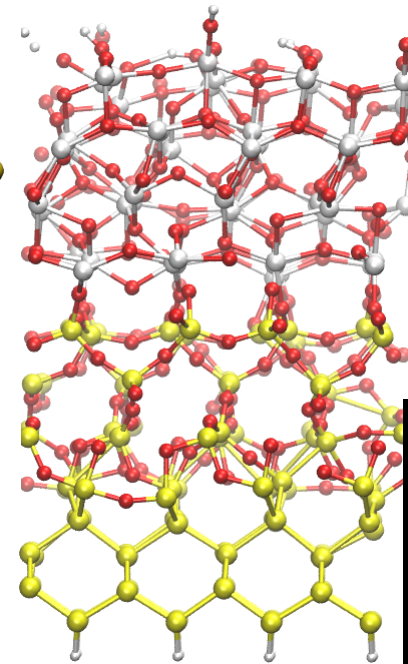


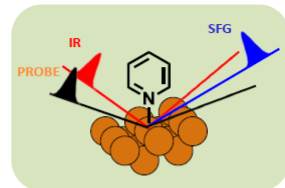
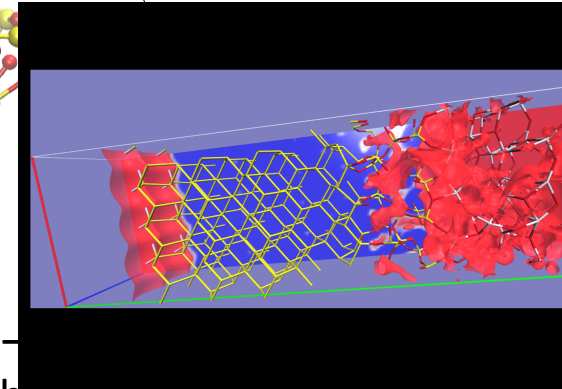
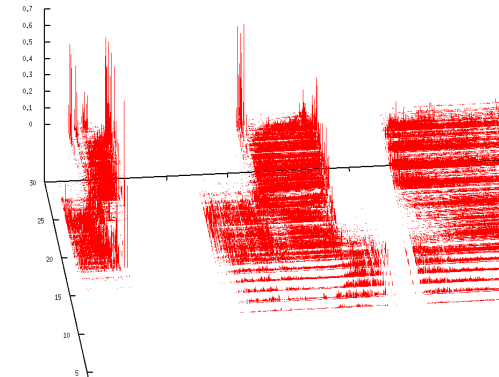
Properties of adsorbed molecules and defects
Simulation – AFM, STM



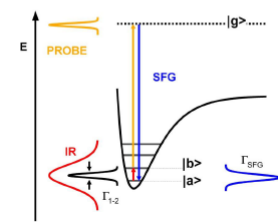
Statistics of defects in
amorphous materials



Complex interfaces –
alignment critical – hybrid functionals



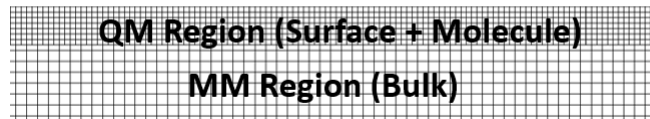
Excited
states &
vibrational
spectroscopy



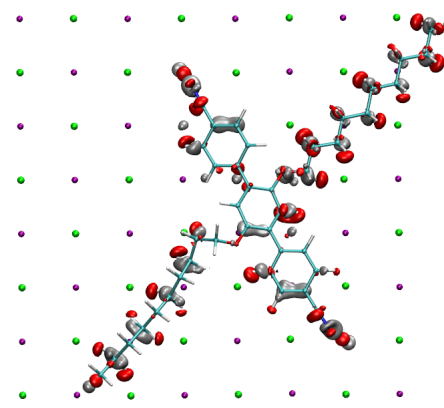
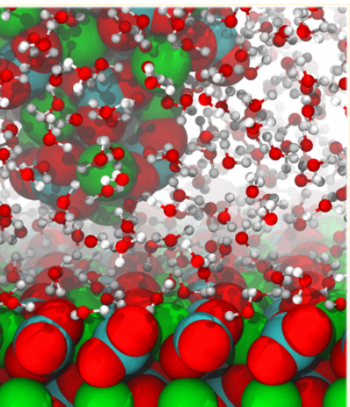
MM Region (Vacuum)

QM Region (Surface + Molecule)

MM Region (Bulk)



In
solution
too!



Molecular assembly

