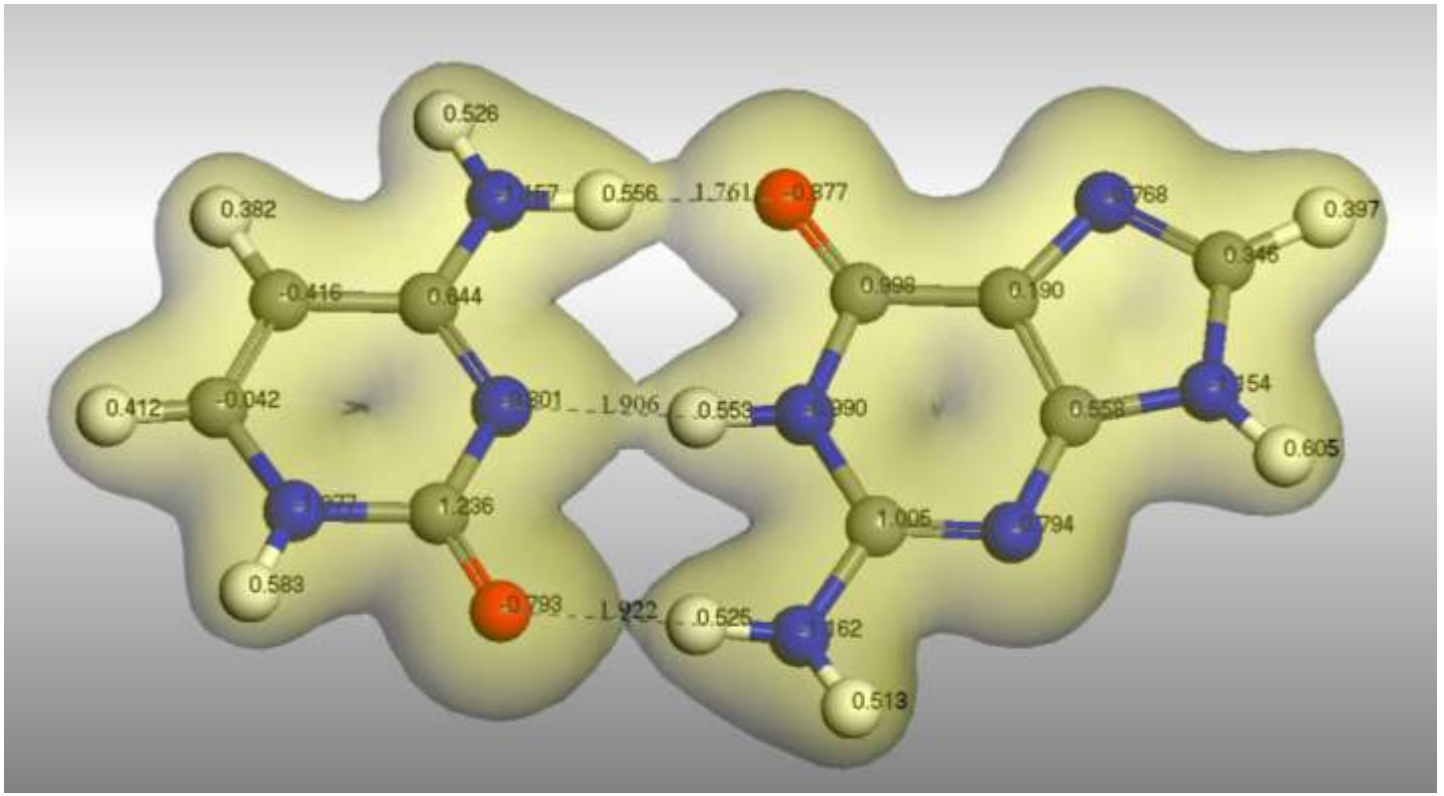
# Andrew Scott – Institute for Materials Research, SPEME

## *Ab-initio* materials modelling – density functional theory

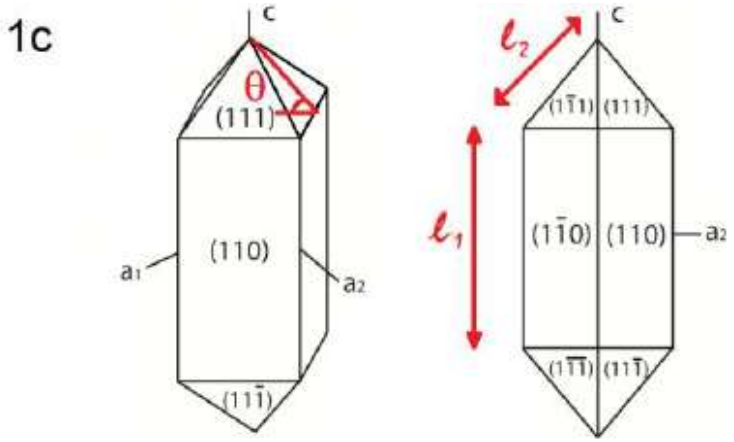
Accurate intermolecular binding/ surface energies
Geometry optimisation – bulk, surface relaxation, phase stability
Data for improved MD potentials e.g. atomic charges, elastic constants

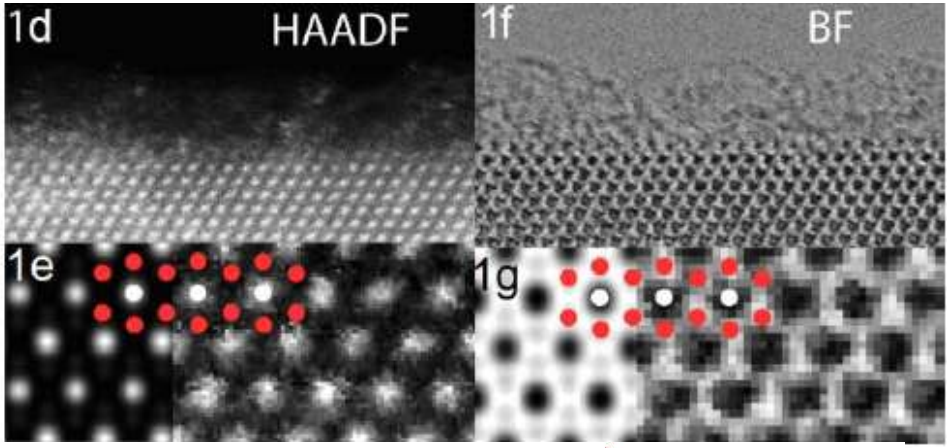


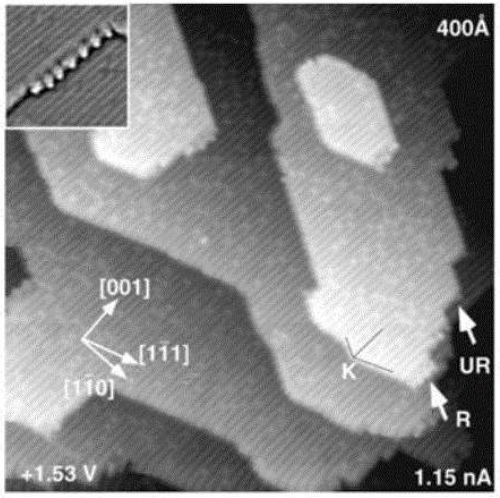

Guanine-cytosine Binding energy: -31.1 kJ/mol

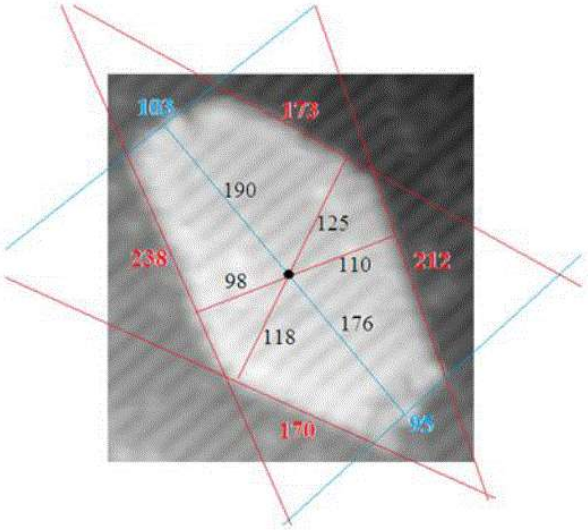
# Surface energies – morphology prediction

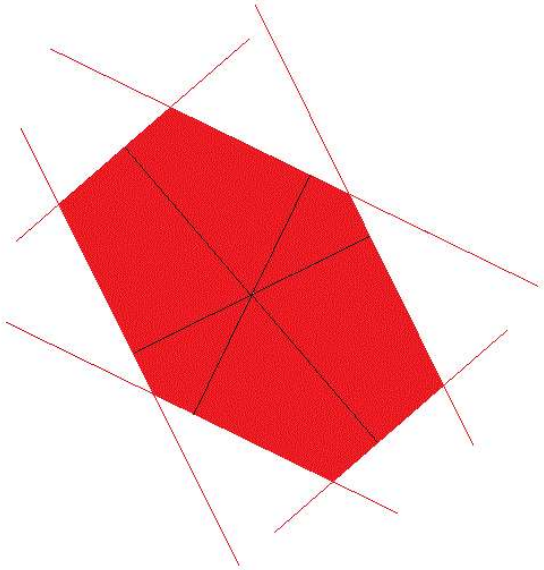
- Trevor Hardcastle



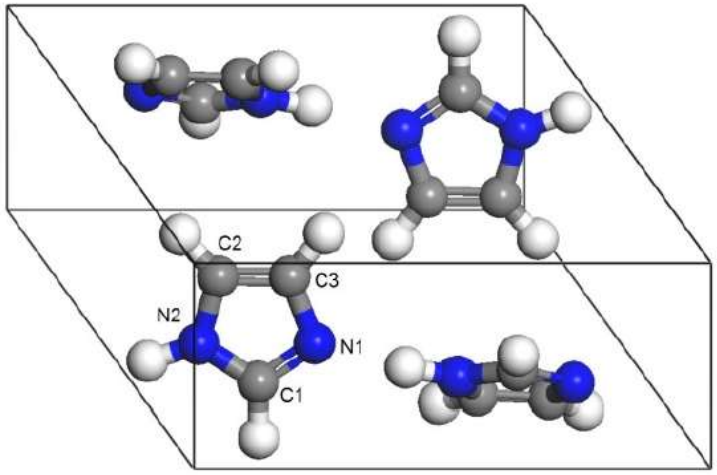
**"inverse" Wulff construction using image dimensions**

**"forwards" Wulff construction using my DFT values**

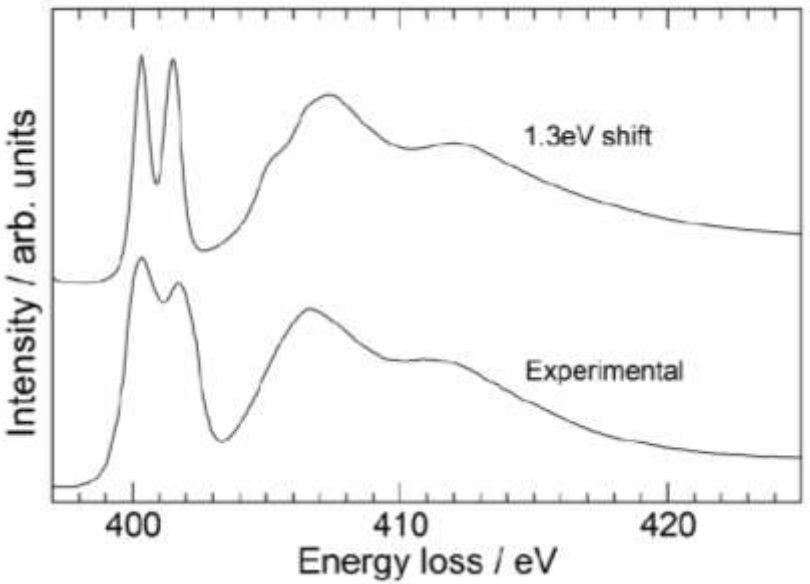
| *Non-polar termination type* | *(110)* | *(100)* | *(101)* | *(001)* | *(111)($TiO_2$)* | *(111)(O)* |
|---|---|---|---|---|---|---|
| $\gamma_{(termination)(vac)}$ /$Jm^{-2}$(2 d.p.) | *0.42 ± 0.08* | *0.62 ± 0.08* | *0.98 ± 0.08* | *1.15 ± 0.08* | *1.33 ± 0.08* | *1.35 ± 0.08* |

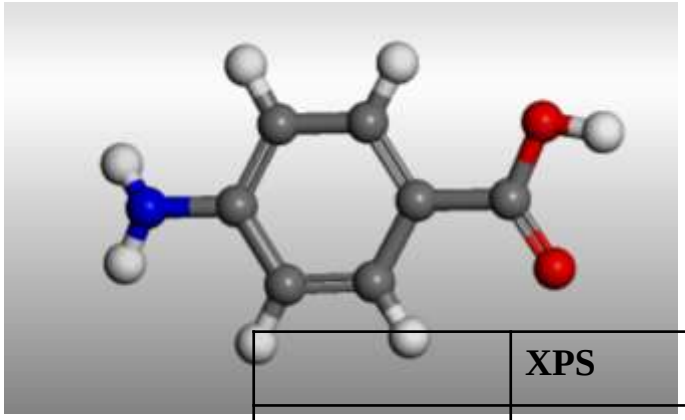
# X-ray absorption near edge structure (XANES/NEXAFS)

- Che Seabourne

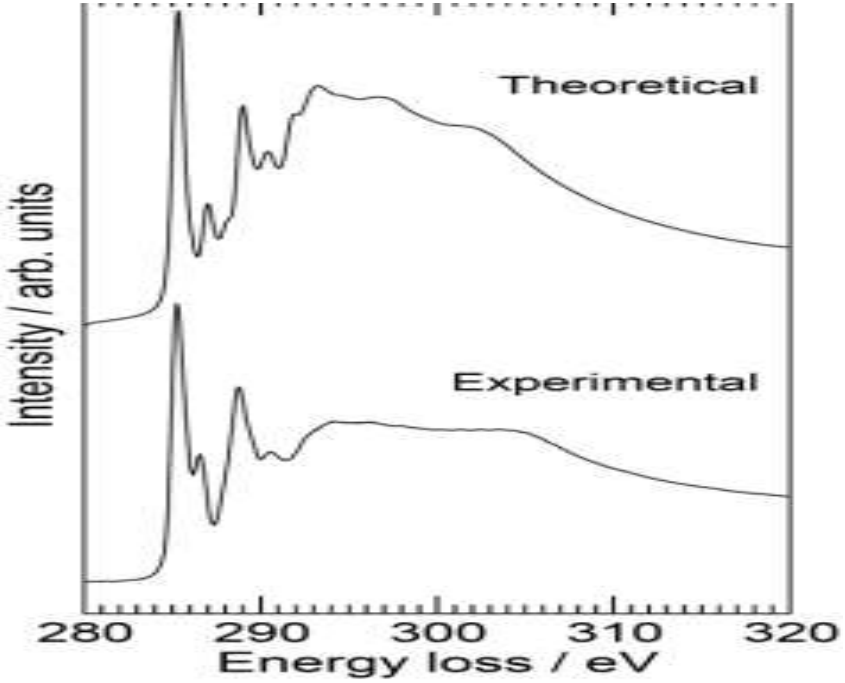



Imidazole



PABA




| | **XPS** | **WIEN2K** |
|---|---|---|
| **C=C** | Baseline | Baseline |
| **C-COOH** | +0.45eV | +0.44eV |
| **C-N** | +1.31eV | +1.75eV |
| **COOH** | +3.96eV | +3.71eV |