Bioorganic & Biophysical Chemistry Laboratory *(PI, Ian A Nicholls)*
- a part of the Linnaeus University Centre for Biomaterials Chemistry

We work with molecular recognition phenomena and the informed design, development and application of functional/biomimetic materials. Areas of application include catalysis, sensing and biomaterials. Our current and projected computational activities include…

Molecular Dynamics:
- primarily for complex mixtures

Quantum Chemistry:
- primarily for small molecule systems

Chemometrics/multivariate statistics:
- Primarily for the study of structure-function relationships where we are using workstation/PC-based software

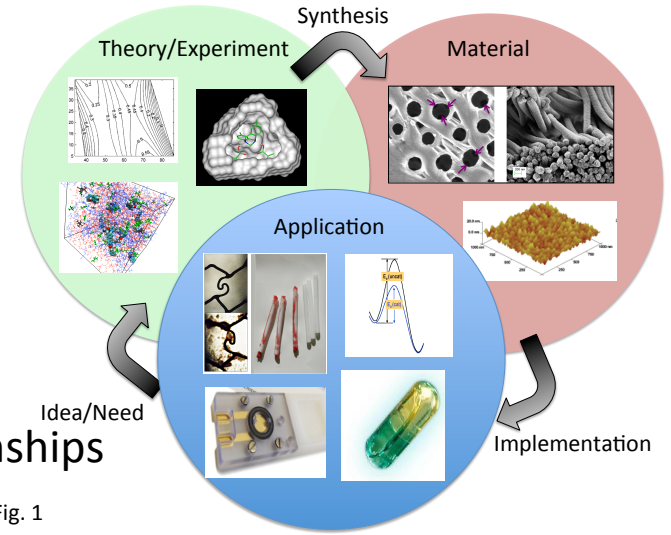

Fig. 1

The BBCL is a medium-size SNIC user (≈50k cpu/annum)
Our **primary local need** today is storage, currently ≈50TB & increasing with 5-10TB/annum
Primary server-based software used: Gaussian 09, AMBER, GROMACS
Support for current projects involving significant volumes of computational studies:
EU 7th framework (2 projects), VR, industry