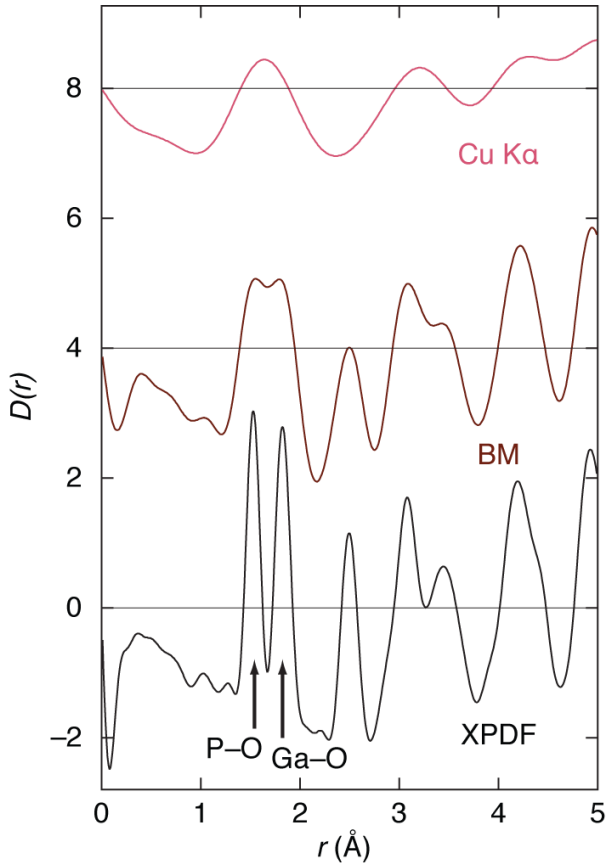
# XPDF

A Dedicated X-ray PDF Beamline
Phase III Beamline Proposal

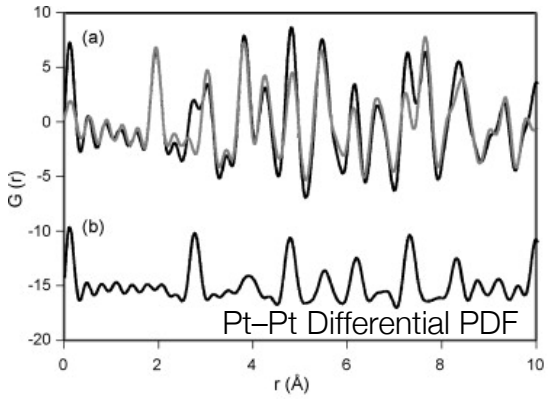
*DISCO Presentation 24 February 2011*

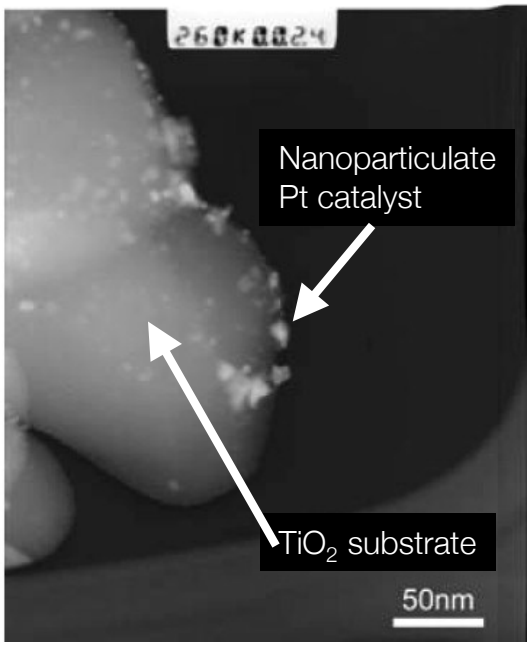
# Pair Distribution Function (PDF)

- Quantitative experimental probe of local structure in materials
- Fourier transform of powder diffraction pattern; gives histogram of interatomic separations
- Quantifies “true” bond lengths, coordination number, dynamics
- Resolution determined by $Q_{max}$ so requires high-energy X-rays
- Applicable to crystals, nanocrystals, amorphous materials, liquids



# Catalysis



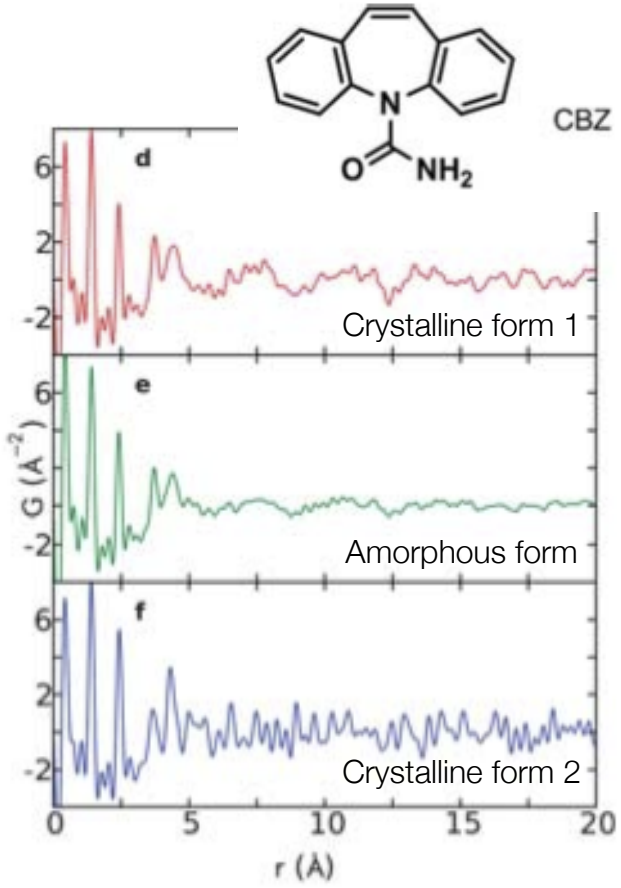




- "Differential PDF" allows structural characterisation of *e.g.* nanoparticulate catalysts mounted on solid substrates
- Rapid PDF analysis allows for *in situ* measurements of local structure changes in real time during catalytic processes
- Model-independent observation of interatomic distances; *cf* EXAFS, NMR

Chupas, Chapman, Chen and Grey, *Catalysis Today* **145**, 13 (2009)

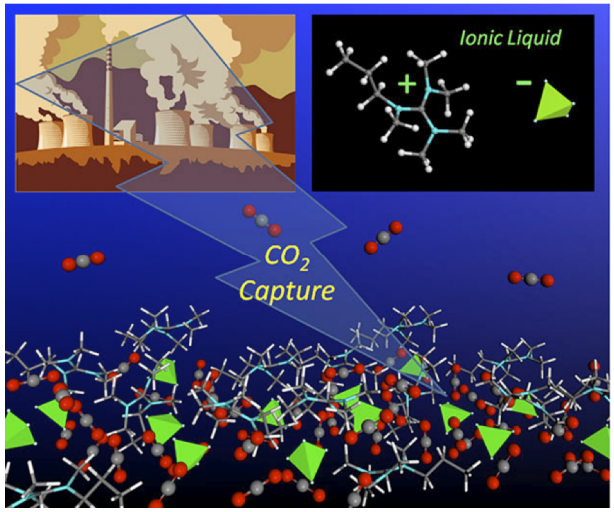
# Health and Pharmaceutics

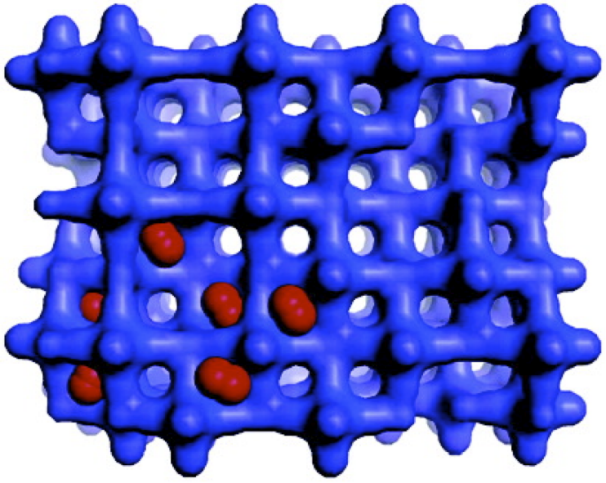
- Structural characterisation of amorphous and nanocrystalline drug materials
- “Fingerprinting” for IP applications
- Determination of impact of processing on solid form of amorphous products
- Tracking of structural changes with time, temperature and %R.H.
- Characterisation of crystallisation pathways in amorphous biomaterials; *e.g.* a-$Ca_3(PO_4)_2$




Billinge et al, *CrystEngComm* **12**, 1366 (2010)

# Energy



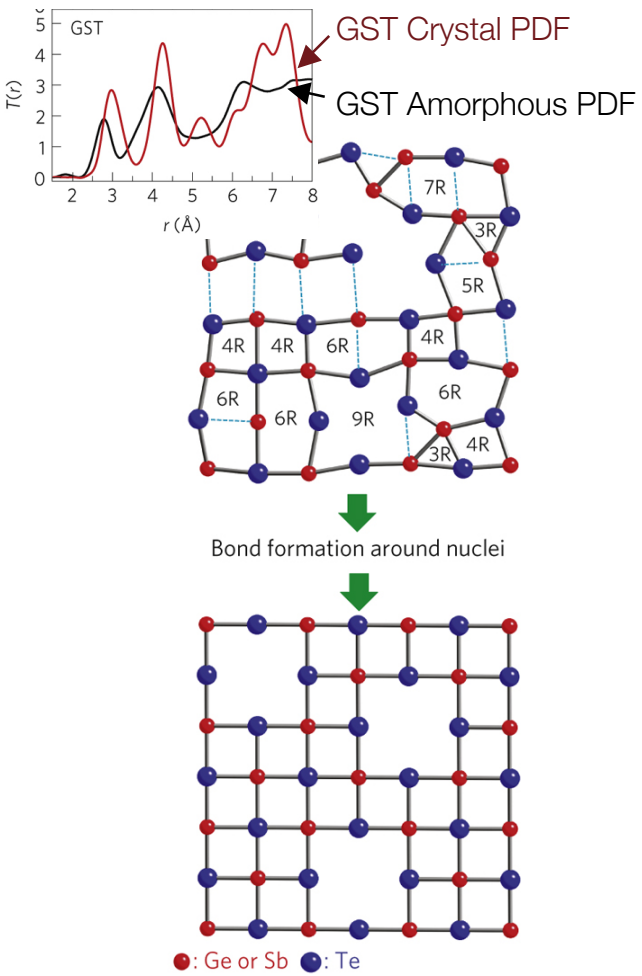



- Gas sorption dynamics and binding site preferences in porous materials
- $CO_2$ capture in ionic liquids
- *In operando* measurement of ion transport mechanisms in battery materials
- Parametric studies under variable temperature, pressure, gas flow, charge/discharge

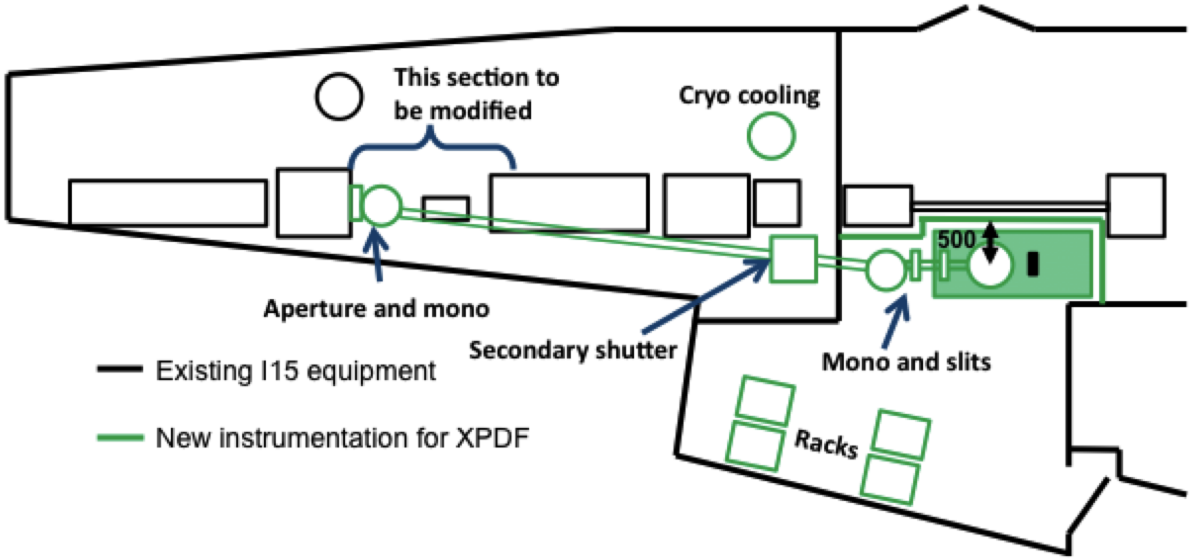
# Digital Economy

- Structure–electronic property relationships in amorphous transparent conducting oxides
- Local structure and dynamics in thin-film ferroelectrics
- Nanoscale disorder in dilute magnetic semiconductors for spintronics
- Amorphous–crystalline transitions in phase change chalcogenides for data storage (*e.g.* DVD-RAM)

Matsunaga et al, *Nature Materials* **10**, 129 (2011)



# XPDF Beamline Design




- Sidestation to I-15 with high-energy beam profile (superconducting multipole wiggler)
- Cost-effective design maximises scientific potential of existing infrastructure
- Range of sample environments; 2D detector for rapid and robust data acquisition

# XPDF Industrial Supporters