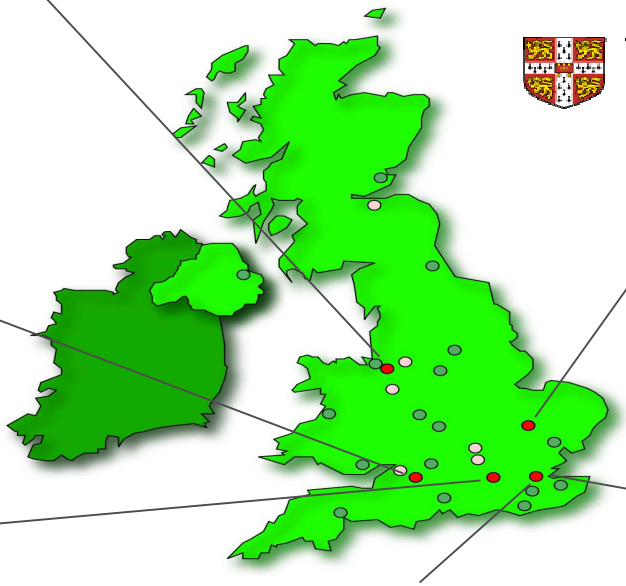
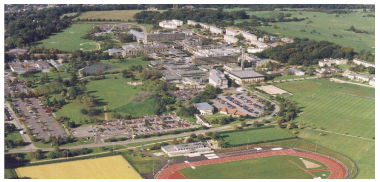
eMinerals Grid Interface

Rik Tyer
Grid Technology Group
Daresbury Laboratory

eMinerals Project





University of
Reading

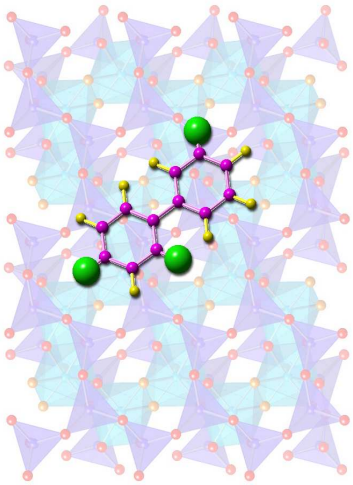
Royal Institution

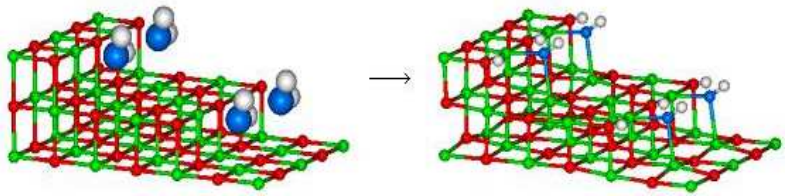
Science Drivers

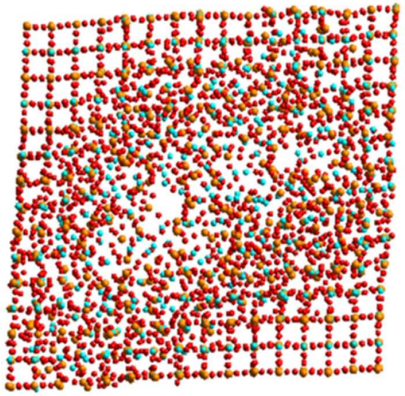
Radioactive waste disposal

Pollution: molecules and atoms on mineral surfaces

Crystal dissolution and weathering

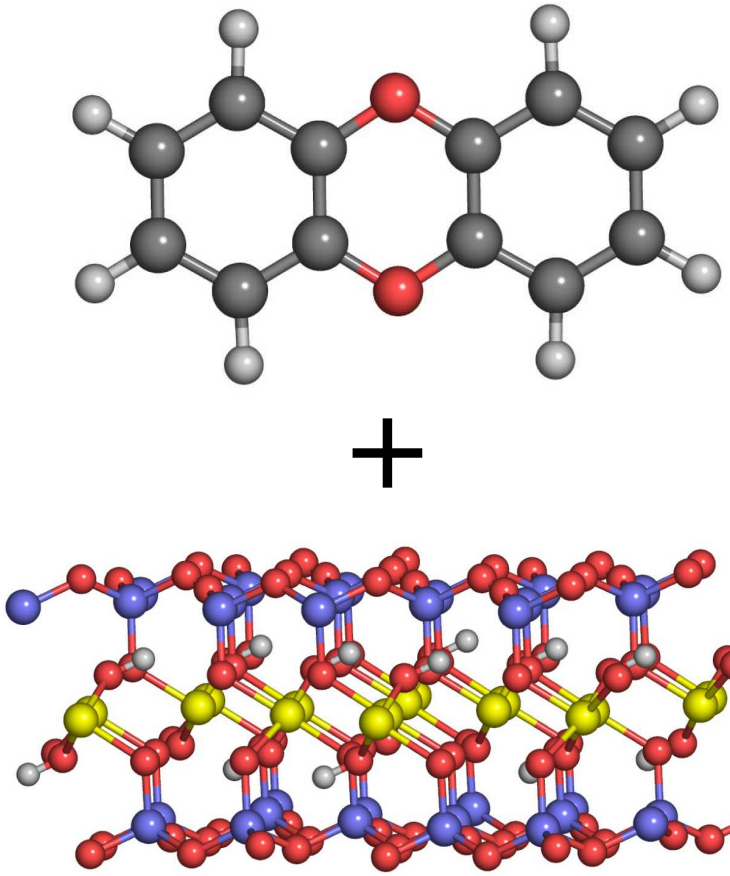


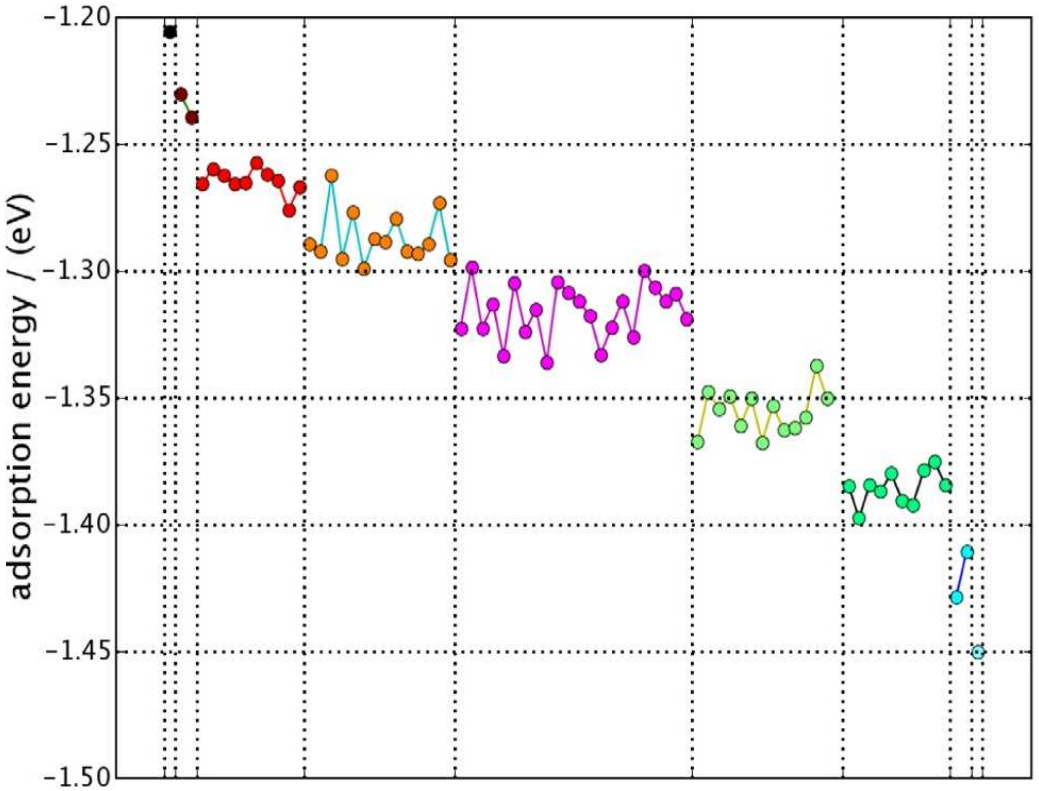




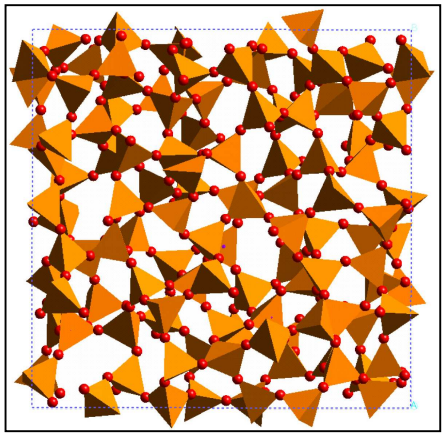
Crystal growth and scale inhibition

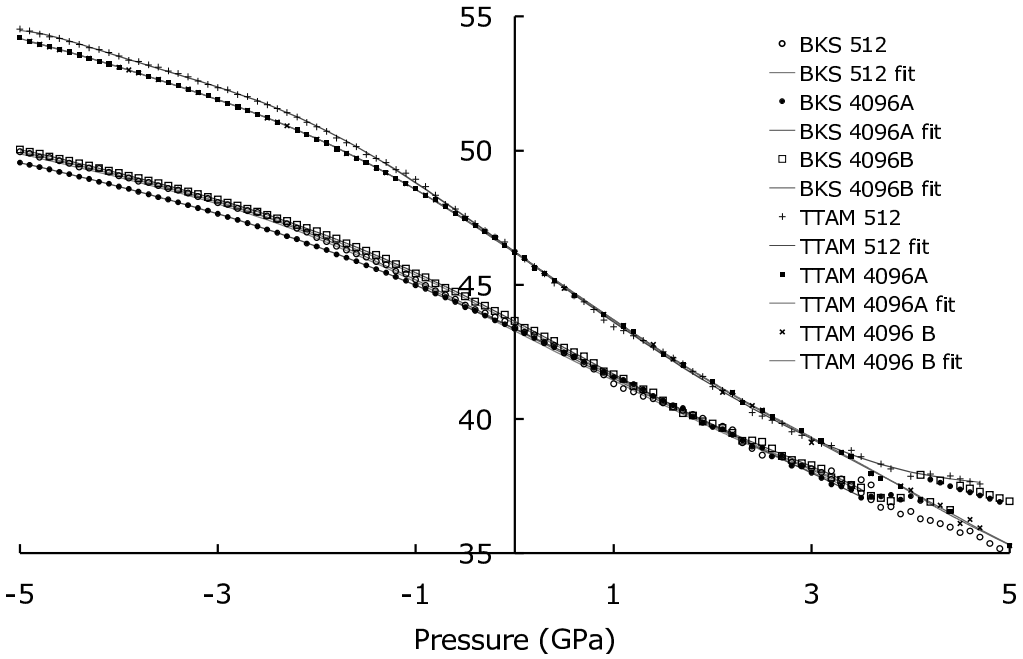
Dioxin molecules on silicate surfaces





Compressibility of amorphous silica





- Simulations of pressure-dependence of amorphous silica
- Volume curve shows that silica gets softer around 2 GPa
- Negative derivative defines the compressibility

Parameter Sweeps

- Grid killer feature
- Periods when require large numbers of processors, interspersed with quiet periods for analysis
- Need single access point to all compute resources
- Need single access point to data
- Really need to use metadata as primary interface to data
- Running large numbers of simulations requires integrated compute, data and metadata functionality

RMCS Overview

- Genuine desktop grid client
- No need for VDT, Globus etc installed locally
- Require:
  - RMCS binaries or client library (web service client)
  - Ability to interact with data grid (SRB) (CLI, GUI, portals, webDAV)
  - Ability to interact with metadata (web service client, portals)
  - Ability to upload proxy to MyProxy server (Java Web Start)
- Should require no firewall configuration
- All sockets client initiated

RMCS Functionality

- Metaschedules
- Download bin and input files

Pre-processing Actions

- Runs simulations (Sequential, MPI or Condor)

Main Job

- Parse output XML for key data
- Upload output files to SRB
- Upload metadata

Post-processing Actions

RMCS Interface

Executable = lmto

pathToExe = /home/rty.eminerals/SIC_20_cml

preferredMachineList = lake.esc.cam.ac.uk grid-compute.leeds.ac.uk dl1.nw-grid.ac.uk-serial

Input = scf

jobType = performance

numOfProcs = 1

Sdir = /home/rty.eminerals/CaCuO2/Lattice

Sget = *

Sput = char_out out fort.41 e-ny output.xml

Queue

Demo – Monte Carlo Simulation

- Want to study phase diagram of a silicate system as a function of temperature
- Will submit 10 simulations with different temperatures to NWGrid machines (DL, Liv, Lancs)
- At the end of the calculation, output files should be archived within the SRB
- Should be able to obtain key results direct from the metadata harvested