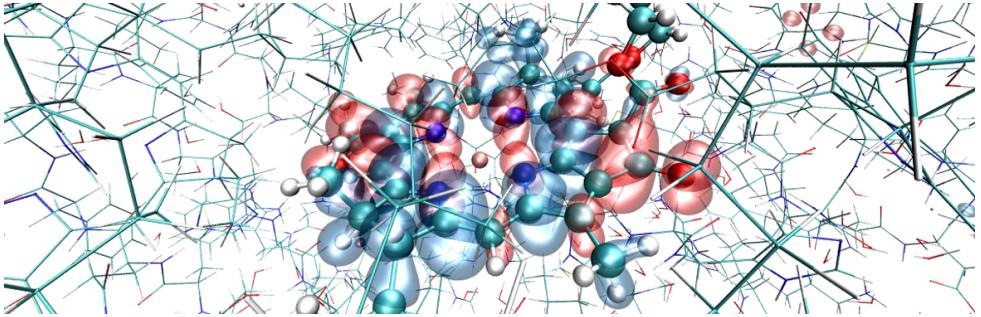
Nanomaterials Simulation



- Hine group: Ab Initio calculations on molecular systems and nanomaterials in complex environments:
- Specialisms: excited states, UV/vis spectroscopy, vibrational spectroscopy, photoemission, core loss etc.
- Linear-Scaling DFT: scalable from tens to thousands of atoms (∼10-20 nm): small molecules to whole proteins, nanocrystals etc

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- Highly parallelisable, but also runs on modest computational resources
- Features as a module in the widely-used Materials Studio package (Dassault Systemes BIOVIA)

Current interests:

- first-principles colour/spectrum prediction
- identification of secondary species in solution by optical spectroscopy
- machine-learned energy surfaces for theoretical spectroscopy (HetSys project)