Researcher Background

Anthony Reilly, FI

- Assistant Professor in Computational Chemistry
- PhD from U. Edinburgh, previous research positions in leading research organisations in UK and Germany
- Chartered Chemist, Member of the Royal Society of Chemistry and Institute of Physics

Research Field

Modelling of molecular materials, developing and applying state-of-the-art computational methods to understand the structure and properties of molecular crystals

- First principles modelling using density-functional theory to understand complex interactions with crystals
- Structural informatics for rapid assessment of stabilities and behavior

Scientific Impact

- > 30 peer-reviewed publications and review articles
- > 900 citations, h-index of 13, two recent publications rated as “Highly Cited Papers” by Web of Science
- 12 invited conference presentations or seminars

Technological Impact

Computational modelling can underpin the design and understand of molecular materials

- Prediction and assessment of the stable solid forms of pharmaceuticals and their properties (e.g. mechanical response, solubility)
- Functional molecular materials with tailored response properties, for applications including sensors and organic electronics