

**1. Title of Case Study:** Topologically directed discovery of functional co-ordination materials

**2. Grant Reference Number or Facility Name:** University of Sussex, Dr George Kostakis, accessing National Crystallography Service, University of Southampton.

**3. One sentence summary:**

**4. One paragraph Summary:** Data from the University of Southampton's National Crystallography Service (NCS) is helping chemists at the University of Sussex address major challenges in synthetic chemistry to produce functional and transformative materials.

**5. Key outputs in bullet points:**

NCS data is enabling:

- transformative multidisciplinary science leading to new knowledge
- new collaborations with chemists to study the properties of compounds
- the training of chemical topological scientists to design and develop new materials that will address the needs of the future industry
- the training of students who will understand the potential application of their research and develop skills to enable them to progress in emerging sectors and traditional industries

**6. Main body text**

Data from the University of Southampton's National Crystallography Service (NCS) is helping chemists at the University of Sussex address major challenges in synthetic chemistry to produce functional and transformative materials.

Dr George Kostakis, Senior Lecturer In Physical/Inorganic Chemistry at the University of Sussex, said: "Our research combines techniques and expertise from inorganic, co-ordination, topology, theoretical and organic chemistry. This Topological Co-ordination Chemistry (TOPOCONIC) approach will broadly systemise the discovery of new functional co-ordination compounds, complementing state-of-the-art techniques to harvest new materials. Our comprehensive programme aims to:

- introduce a conceptually different synthetic methodology exploiting compositional parameters
- systemise and topologically rational assemble co-ordination compounds
- correlate topology and property relationships with applications in interdisciplinary fields

This research will create the necessary background to develop new methodologies for materials with specific properties in areas as disparate as catalysis, biochemistry and molecular magnetism. It has the potential to increase the storage capacity/memory of devices, and improve and lower the costs of drugs.

"We work with compounds whose synthesis is complicated and attempts at the systemisation of these compounds have been very sparse. If we could elucidate the mechanisms and processes to make these compounds more generally available, it would be very beneficial. We could overcome the challenges of a reproducible synthesis, controlling the shape and size, as well as the fine-tuning of chemical and physical properties.

The Kostakis group have set up Polynuclear Inorganic Clusters Database as part of this approach, x-ray crystallography provides a lot of detailed structural information for this project.

Dr Kostakis says "Working with the NCS at Southampton is integral to our research. The materials we are investigating can be weakly diffracting, and the NCS has all of the relevant equipment and expertise to provide a full characterisation of the material which is essential for our project.

"We have a really good relationship with the NCS. We have been using their services for the past four years and they know what we are trying to achieve and what they can do to help facilitate this. They are in constant contact as they collect and solve datasets."

The collaboration between the Kostakis Group and the NCS has been productive with 9 co-authored papers as of the date of publication.

**7. Names of key academics and any collaborators:**

Manchester (EPR)

Akien (Lancaster 89Y-NMR)

Spivey (Imperial College)

Arseniyadis (Queen Mary's)

**8. Sources of significant sponsorship (if applicable):**

£92,400 EPSRC EP/MO23834/1, Feb 2015

**9. Who should we contact for more information?**

Dr George Kostakis, University of Sussex ([G.Kostakis@sussex.ac.uk](mailto:G.Kostakis@sussex.ac.uk))

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**To keep in mind:**

- The sentence and paragraph summaries should be able to stand alone – they are the sort of things that can be put on a slide or in a `highlight box`, accompanied by a picture or figure
- For the main case study, break the text into paragraphs: What, How, Why
- Keep to a clear story in simple language for a general audience
- Take a wide perspective on real world impact
- Answer the “so what?” question
- Explain how EPSRC funding has made this breakthrough possible
- Include numbers, but leave out technicalities
- Include pictures that capture the imagination of the audience
- Avoid jargon and acronyms