PhD PROJECT PROPOSAL

## **PhD Project Title**

Exploring Topological States in 2-D Magnetic Materials

## **PhD Supervisory Team**

Principal Supervisors: Dr Lucy Clark, [l.m.clark@bham.ac.uk](mailto:l.m.clark@bham.ac.uk), Materials Chemistry, School of Chemistry

Co-supervisor: Prof. Giovanni Costantini, [g.costantini@bham.ac.uk](mailto:g.costantini@bham.ac.uk), Costantini Group, School of Chemistry

Industrial Supervisor: Dr Vladimir Korolkov, Park Systems

Associated Academic: Dr Stefano Ruspani, [stefano.rusponi@epfl.ch](mailto:stefano.rusponi@epfl.ch), Laboratory of Nanostructures at Surface, Institute of Physics, EPFL.

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## **Project Abstract**

## Theoretical physics predicts that the properties of two-dimensional (2D) materials are

## entirely distinct from the behaviour we understand from the three-dimensional world

## around us. A well-known example is the two-dimensional material graphene. However,

## while graphene has many remarkable materials properties, it is not intrinsically magnetic.

## Magnetic materials form the basis of many modern-day technologies, yet the discovery of

## two-dimensional magnetic materials remains an outstanding research challenge that could

## transform science and technology. This PhD project aims to overcome this challenge by

## realising long-sought models of 2D magnetism in an emerging class of 2D—metal-organic

## nanosheets—and will uncover their exotic materials properties using state-of-the-art

## surface science techniques.

## **Detailed Project Description**

**Research Background and Aims**

Topological design predicts that the properties of 2D magnetic materials are entirely unique to the classical magnetic states of matter that are familiar in three-dimensional materials. This topological theory creates an incredible impetus for experimental materials research to discover realisations of 2D materials and to develop the techniques required to uncover their unique behaviour. An extraordinary experimental breakthrough in this regard came in 2004 with the discovery of graphene.1 However, while this two-dimensional material has many remarkable physical properties, it is not naturally magnetic. Thus, there remained the tantalising research challenge of discovering a two-dimensional magnetic material that may realise the exotic phenomena predicted by topological design.2 That was until 2017, when two landmark studies reported the detection of intrinsic ferromagnetism in atomically thin layers of two chromium-based inorganic materials, CrI3 and Cr2Ge2Te6.3,4 Like graphene, these materials are composed of van der Waals coupled layers that, in theory, can be mechanically exfoliated into atomically thin sheets. By following the temperature-dependent magnetic response of these exfoliated materials, an intrinsic layer-dependent magnetic behaviour was uncovered, providing the first experimental insight into two-dimensional magnetic materials.3,4 While these studies demonstrate promise for controlling and detecting magnetism in two-dimensions, the chemical nature of the materials investigated, and the magnetic models developed to describe them, are severely limited. Most notably, these inorganic materials are unstable in the single-layer limit, ultimately restricting their potential for incorporation into novel devices and applications.

In this PhD project, you will work to overcome these timely research challenges by diversifying the chemical nature of magnetic materials that can be exfoliated to the 2D limit, preparing and analysing on-surface two-dimensional model systems and developing the toolkit needed to characterise their structure and properties. In particular, materials that are versatile from the perspectives of chemical tunability and stability upon exfoliation are especially needed. Metal-organic nanosheets (MONs) are an emerging class of materials that meet these requirements.5,6 Building on recent developments at the University of Birmingham, you will aim to synthesise novel magnetic MONs and understand how their structural and magnetic behaviours evolve on approaching the two-dimensional limit. A further essential requirement for the success of this project is the ability to characterise these materials where “every atom counts”, with advanced methodologies specifically developed for two-dimensional materials at the ultra-low concentration limit. In this regard, you will be integrating your experimental activity at the University of Birmingham with work done at international synchrotron central facilities.

**PhD Skills and Training**

This PhD will provide skills training in a wide variety of state-of-the-art materials synthesis and characterisation methods. This includes the solution synthesis of magnetic metal-organic framework materials, their exfoliation to form 2D metal-organic nanosheets and the characterisation of their bulk structure and properties by diffraction and magnetometry. These will be complemented by skills in the on-surface fabrication of two-dimensional MONs under highly controlled ultrahigh vacuum conditions and their *in-situ* characterisation by means of scanning tunnelling microscopy (STM) and spectroscopy. A further important aspect will be the development of methods needed to detect the structure and properties of various layered magnetic materials in the 2D limit. This includes atomic force microscopy (AFM, both standard and high-resolution) for determining the morphology and periodicity of the layers, surface X-ray diffraction (SXRD) for defining their two-dimensional unit cells, X-ray photoelectron spectroscopy (XPS) to establish their composition, relative stoichiometry and chemical state and X-ray magnetic circular dichroism (XMCD) for determining the spin and orbital magnetic momentum of the magnetic elements.

**Fit to the CDT in Topological Design**

The 2016 Nobel Prize for Physics was awarded to Thouless, Haldane and Kosterlitz for their theoretical discoveries of topological phase transitions and topological phases of matter. Put simply, Thouless, Haldane and Kosterlitz developed new theories that predict highly unusual behaviour in materials when their constituent atoms are constrained to only one- or two-dimensions. In particular, by using topology, they showed that the physics of low-dimensional materials is entirely different to our three-dimensional world. This project utilises these seminal developments in topology to design and characterise novel realisations two-dimensional magnetic materials, in which low-dimensional magnetic interactions are predicted to give rise to exotic and novel materials properties.

**Research Team and Collaborations**

You will work collaboratively across the Clark and Costantini research groups to develop a new research initiative in topological materials design and characterisation. The two supervisors are both based in the School of Chemistry of the University of Birmingham but have highly complementary backgrounds (Clark in Chemistry and Material Science, Costantini in Physics and Surface Science) and expertise. The research focus in the Clark Group is on the design, synthesis and characterisation of novel quantum materials. The Clark group has strong research connections to leading international central research facilities, including the ISIS Neutron and Muon Source and the Institut Laue-Langevin. The Costantini Group has recently joined Chemistry Birmingham transferring their 20+ years of expertise in molecular nanoscience at surface and high-resolution scanning probe microscopy. Their long-standing collaborations with several European synchrotron facilities (Diamond, ELETTRA, ESRF), with world leaders in molecular and atomic-scale experimental magnetism (Rusponi, EPFL) and with theoretical colleagues using density functional theory calculations to describe nanomagnetic materials (Maurer, Warwick), will be of central importance for this project.

**Candidate Requirements and Expectations**

Candidates must have a First Class or Upper Second undergraduate degree in Chemistry, Physics or Materials Science. Candidates should also have an enthusiasm for interdisciplinary experimental materials research as well as a capacity to develop an advanced understanding of the underpinning theory motivating this work and the experimental methods to be used.

**References**

1 KS Novoselov et al., Science 306, 666 (2004)

2 JM Kosterlitz and DJ Thouless, J. Phys. C: Solid State Phys. 6, 1181 (1973)

3 C Gong et al., Nature 546, 265 (2017)

4 B Huang et al., Nature 546, 270 (2017)

5 DJ Ashworth and JA Foster, J. Mater. Chem. A 6, 16292 (2018)

6 J López-Cabrelles et al., Nat. Chem., 10 1001 (2018)