Experimental report

02/05/2022

Proposal: 5-41-1172 **Council:** 4/2021

Title: Novel magneto-electric order parameter in cupric oxide.

Research area: Physics

This proposal is a new proposal

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Samples: CuO

Instrument	Requested days	Allocated days	From	To
D3 CPA	4	9	14/05/2021	17/05/2021
			02/06/2021	07/06/2021
			07/06/2021	08/06/2021
IN20 CPA	4	0		
IN22 CPA	4	0		

Abstract:

In condensed matter systems, the atoms, electrons or spins can sometimes arrange themselves in ways that result in unexpected properties but that cannot be detected by conventional experimental probes. Several historical and contemporary examples of such hidden orders are known and more are awaiting discovery, perhaps in the form of more complex composite orders. The aim of this proposal, is to study a new type of order parameter in CuO, which arises from spontaneous long-range ordered arrangement of local magneto-electric moments. We propose to detect these ordered moments by measuring full polarization matrices with spherical neutron polarimetry. With the strong support from theoretical and computational predictions, the identification of this new type of order, may herald a new way to classify condensed matter systems.

The proposed study concerns a new type of order parameter, arising from the ordered arrangement of magneto-electric (toroidal) moments. These toroidal moments (t), composed from a composite of magnetic and electric dipoles, can arise in materials that lack both time-reversal symmetry (TRS) and spatial-inversion symmetry (IS). The dynamic ordering of magneto-electric multipoles has been proposed as a candidate order parameter of under-doped cuprates in the pseudo-gap phase. As such, the study of these toroidal moments, and their long-ranged order, might shed light on the mechanisms that underpin high-TC superconductivity.

Before investigating the under-doped cuprates, we propose first to consider a simpler system, CuO, which is a main constituent in the synthesis of these cuprates. The Cu ion resides on the non-centrosymmetric 4a Wyckoff site of the monoclinic Cc space group and displays collinear magnetic order in the AFM1 phase with a propagation vector q = (½, 0, –½) below T = 213. As such, the Cu ions fulfil both of the necessary conditions to possess toroidal moments since TRS and IS are broken.

Our theory partner (N. Spaldin, ETHZ) pioneered the use of a computational approach to model the toroidal moment in CuO. This full-electron code (ELK) provides for a comprehensive description of the hybridization of the electrons in CuO. The calculations predict that the toroidal moments display anti-ferro toroidal order, with a propagation vector of q = (½,0,-½), and, for the first time, provide estimates of the toroidal moment length and orientation.

Guided by these calculations, we performed spherical neutron polarimetry (SNP) on single crystals of CuO. Our measurements are indicative of the magneto-electric moments not only on the Cu site but also on the O site. These SNP measurements were performed on the D3 diffractometer and were not possible if not for the improved flux on the OrientExpress Laue diffractometer, which allowed for the alignment of the monoclinic single crystal.