Invited Lecture

Modular metal-organic magnets: structure informed design

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Metal-organic magnets offer unique opportunities for control over magnetic function, as chemical functionalisation of the framework structure allows for tuning of the functional behaviour. This is particularly true for van der Waals materials, where the chemical flexibility permitted by the organic component allows for a diversity of structure and function not easily realisable in inorganic atomic layered materials. I will highlight in particular our work on the family of layered metal organic magnets $MCl_2(L)$ comprising metal halide chains connected by a molecular ligand (pyrimidine, 2,1,3-benzothiadiazole). This platform allows us to realise a range of different properties, from routes towards the Haldane S=2 quantum chain[1] to controllable non-collinear ferromagnetism [2].

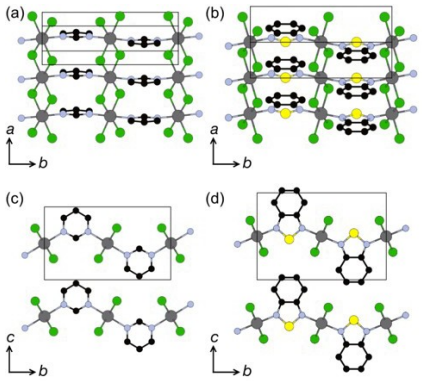

Figure 1. Structure of MCl_2L van der Waals metal-organic magnets (a,c) L = pyrimidine, (b,d) L = 2,1,3-benzothiadiazole

Crystallography is a critical tool for designing new metal-organic magnets: as well as guiding the assembly of desired structural motifs, neutron scattering is invaluable the insights it provides in the magnetic behaviour of metal-organic magnets. It gives otherwise challenging to obtain insights into both the ground states, from Bragg scattering, and interactions of magnetic materials, from modelling of magnetic diffuse scattering and powder inelastic scattering.

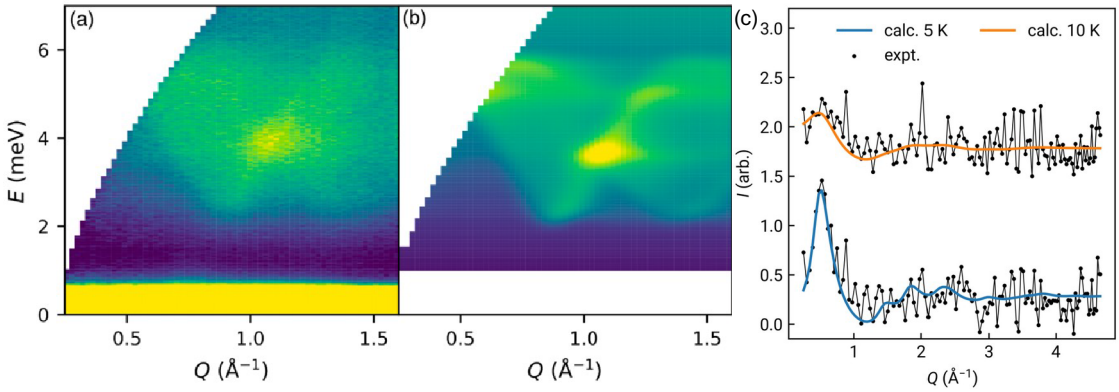

Figure 2. Inelastic powder neutron spectrum of $CrCl_2$(pyrimidine): (a) experiment and (b) linear spin wave calculations [1]. (c) Reaction field modelling of magnetic diffuse scattering in of $FeCl_2$(2,1,3,benzothiadiazole) [2].

[1] J. Pitcairn *et al.*, *J. Am. Chem. Soc.*, **145**, 1783 (2023).

[2] J. Pitcairn *et al.*, *ChemRxiv* DOI:10.26434/chemrxiv-2024-nvj38.

[3] E. N. Bassey *et al.*, *Inorg Chem*, **59**, 11627 (2020).

[4] M. Geers *et al.*, *Chem. Sci.* **14**, 3531 (2023).