Recent scientific highlights from the Pelican user programme

Richard A. Mole and Dehong Yu

The direct geometry, time-of-flight spectrometer Pelican has been in the user programme since October 2014 at the OPAL research reactor at the Australian Nuclear Science and Technology Organisation (ANSTO). Situated on the cold guide CG1, Pelican is suited to measuring low energy excitation's from varying materials. This encompasses phenomena that are as diverse as the diffusion of water in clays to the observation of crystal field splitting in rare earth magnets.

Phonon density of states of titanium oxides

Magneli titanium oxides with stoichiometry Ti_nO_{2n-1} have been extensively studied in view of there potential for photocatalytic, thermoelectric and photothermal applications. This work used a variety of techniques, including inelastic neutron scattering and DFT calculations to determine the relationship between the structure of the oxygen defects and the correlation with these varying physical properties. The combined use of phonon density of stat states measurements and DFT calculations allows modes from specific components eg Ti_3O_5 to be quantified.

Manipulation of planar oxygen defect arrangements in multifunctional magneli titanium oxide hybrid systems: from energy conversion to water treatment;

Yichen Liu, Jack Yang, Sean Li, *et al* Energy and Environmental Science, 2020, DOI: 10.1039/d0ee02550j

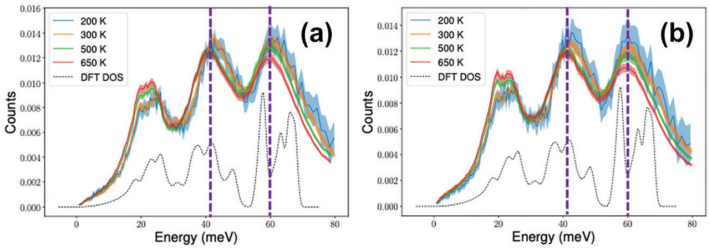

Fig1: Temperature dependent phonon density of states for (a) 71.6 % Ti_2O_3-28.4 % Ti_3O_5 and (b) 70.3 % Ti2O3-29.3 % Ti_3O_5 – 0.5 % TiO with the total DFT calculation also shown.

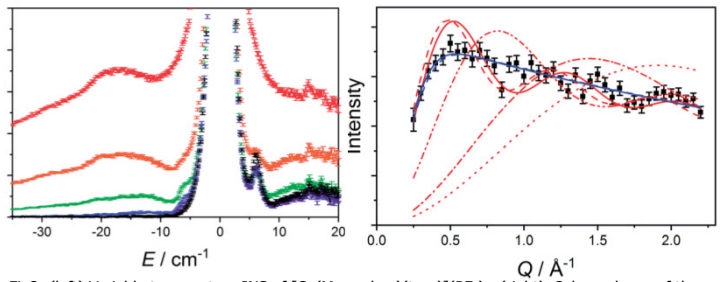

Fig2: (left) Variable temperature INS of [Co(Me_4cyclam)(trop)](PF_6). (right) *Q* dependence of the 6.0(4) cm^{-1} transition with fits to varying exchange models shown.

Transition metal radical coupling.

Many recent works have looked at the inclusion of organic radicals in to the design of single molecule magnets and molecular qubits. However the nature of the coupling is often not trivial especially in the case of metal centers with significant single ion anisotropy. In this work inelastic neutron scattering was used alongside complimentary techniques such as EPR, magnetic susceptibility and *ab intio* calculations. Despite the use of a hydrogenous sample, we were able to observe magnetic excitations and examine the Q dependence of these. This allowed the determination of the effect of intermolecular interactions.

Single-ion anisotropy and exchange coupling in cobalt(II)-radical complexes: insights from magnetic and *ab intio* studies

Gemma Gransbury, Alessandro Soncini, Colette Boskovic, *et al. Chemical Science* 2019, **10**, 8855

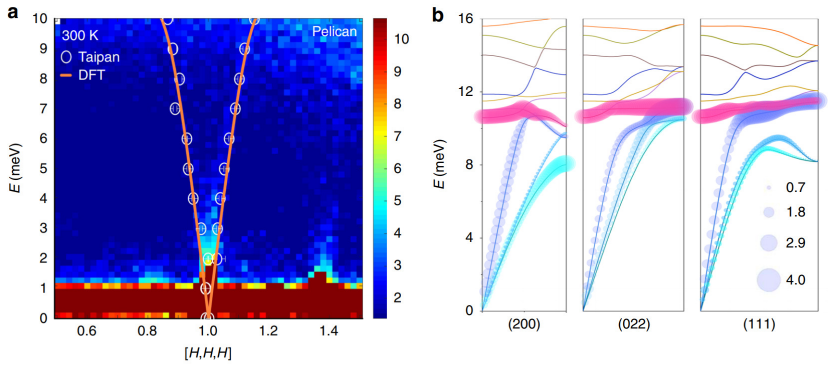

Fig2: (left) Phonon dispersion of CuP_2 obtained using Pelican along the [H, H, H] direction of the Brillouin zone **G** = (1 1 1) Right: Calculated phonon dispersions of Brilliouin zones **G** =(2 0 0), **G** = (0 2 2), **G** = (1 1 1).

Phonon measurement in single crystal CuP_2

Materials with low thermal conductivity are desirable for a great variety of applications such as thermal insulation, phase transition memory devices and thermoelectric energy conversion. In this work the mechanism for the low thermal conductivity in Cu_2P was studied systematically using inelastic neutron scattering and lattice dynamics calculations. The origin of these physical properties was demonstrated to be due to the copper atoms participating in a dimer rattling mode. These strongly anharmonic modes strongly scatter the longitudinal accoustic phonons and lead to anti-crossing phenomena.

Dimer rattling mode induced low thermal conductivity in an excellent acoustic conductor

Ji Qi, Dehong Yu, Bing Li *et al. Nature Communications,* 2020, **11**, 5197

Magnetic Frustration

The nature of quantum spin liquids is a long standing topic in condensed matter physics. The sample $KCu_6AlBiO_4(SO_4)_5Cl$ is an example of a novel frustrated system on the so-called square-kagome lattice.

This work utilised a range of experimental techniques to probe the magnetic properties of this lattice. Inelastic neutron scattering was obtained on several spectrometers, including Pelican at ANSTO. The Pelican experiment was performed using the dilution insert, allowing temperatures of 50 mK to be achieved. These experiments showed that even at these lowest temperatures, the spectrum remains gapless

Gapless spin liquid in a square-kagome lattice antiferromagnet

Masayoshi Fujihala, Katsuhiro Morita, *et al, Nature Communications*, 2020, **11**, 3429

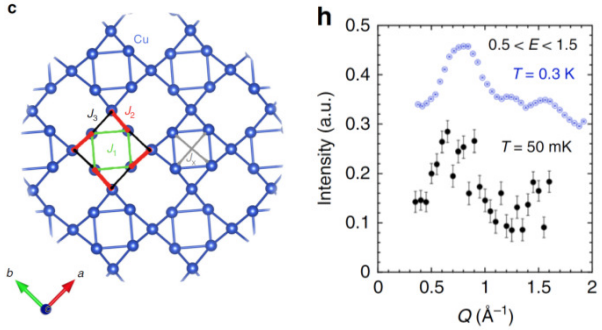

Fig2: (left) Proposed magnetic exchange lattice of $KCu_6AlBiO_4(SO_4)_5Cl$. (right) Q dependence of the INS measured at 0.3 K (AMATERAS) and 50 mK (Pelican).

+61 2 9717 7271 richard.mole@ansto.gov.au www.ansto.gov.au