

## MS20 Electric, opto-electronic and magnetic properties from elastic and inelastic scattering plus properties of materials from quantum crystallography

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Tuning the band structure and Van Hove singularity in  $\text{Sr}_3\text{Ru}_2\text{O}_7$  via isovalent out-of-plane Ba doping

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### Abstract

The orthorhombic  $n = 2$  Ruddlesden-Popper compound  $\text{Sr}_3\text{Ru}_2\text{O}_7$  (structure see Fig. 1a) is a prime example of a strongly correlated oxide, displaying phenomena associated with a quantum critical end point and the formation of complex electronic phases [1,2] at high magnetic fields. The physics of this material is associated with an underlying Van Hove singularity in the band structure (a point at which, in general terms, there is a singularity in the density of states and the Fermi surface undergoes a topological transition, e.g. by different Fermi surfaces touching) [3]. Tuning the properties of  $\text{Sr}_3\text{Ru}_2\text{O}_7$  has been pursued through a number of strategies including magnetic field, pressure, uniaxial strain and doping.

Here, we utilise isovalent Ba doping on the Sr sites as a chemical pathway to expand the lattice and increase the tolerance factor, driving the system closer to the tetragonal aristotype structure (Fig. 1b). Being an out-of-plane dopant, it is expected to minimally affect impurity scattering and thereby transport. Through detailed magnetisation and specific heat measurements, we have discovered a shift towards  $T = 0$  K of the low-temperature specific heat peak known for the  $x = 0$  compound  $(\text{Sr}_{1-x}\text{Ba}_x)_3\text{Ru}_2\text{O}_7$ . This suggests the Van Hove singularity crossing the chemical potential at approximately  $x = 0.08$ , with a subsequent sharp decrease in the density of states. We have investigated this further using high resolution neutron diffraction to probe the link between the crystal and electronic structure in this intriguing set of materials, allowing precise structure-property relationships to be obtained.

We will discuss the details of this tuning of the band structure via structural distortions. In particular we will show how such tuning can provide a clear pathway to increasing the strength and impact of the Van Hove singularity on the physics of  $\text{Sr}_3\text{Ru}_2\text{O}_7$ , and by extension Ruddlesden-Popper ruthenates in general [4].

### References

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