

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

MS20-01

Accessing the electronic structure and magnetism of linearly coordinated transition metal dopants with X-ray dichroism and resonant inelastic scattering

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### Abstract

Lithium nitride ( $\alpha$ -Li<sub>3</sub>N) is proven to be an excellent high symmetry (P6/mmm) host crystal to investigate the single-ion magnetism of linearly coordinated transition metal dopants [1]. Dopants, from Mn(I) through to Cu(I) can be hosted, occupying a linearly coordinated position between nitride ions (figure 1). The basic magnetic properties of the transition metal dopant series include remarkably large easy-plane (Mn, Co) and easy-axis (Fe and Ni) magnetic anisotropy[2]. Fe doped lithium nitride exhibits a magnetic coercivity field exceeding many rare-earth-based permanent magnets with a hysteresis that persists up to 16 K[3]. The magnetism of the series is found to be strongly influenced by 3d<sub>z<sup>2</sup></sub>-4s hybridisation (figure 2). Direct access to 3d-4s mixing and metal-ligand bonding via  $\pi$  and  $\delta$  channels can be resolved by X-ray absorption and magnetic circular dichroism for the late transition metals. However, for Fe, overlapping multiplet excitations inhibit clear spectral assignment. It is only via high-energy resolution 2p3d resonant inelastic scattering X-ray scattering measurements that access to 3d<sub>z<sup>2</sup></sub> mixing enhanced 4s excitations can be observed in Fe doped lithium nitride. The results provide a comprehensive interpretation of the electronic structure, bonding and magnetism of linearly coordinated single-ion magnets. Challenges associated with the precise study of single-ion dopants are shown to be ameliorated by the element sensitivity of X-ray absorption and inelastic scattering.

### References

- [1] M. S. Huzan, et al. Chem. Sci., 2020, 11, 11801.
- [2] A. Jesche, et al. Phys. Rev. B 2015, 91, 18040(R).
- [3] A. Jesche, et al. Nat. Commun., 2014, 5, 3333.

Figure 1

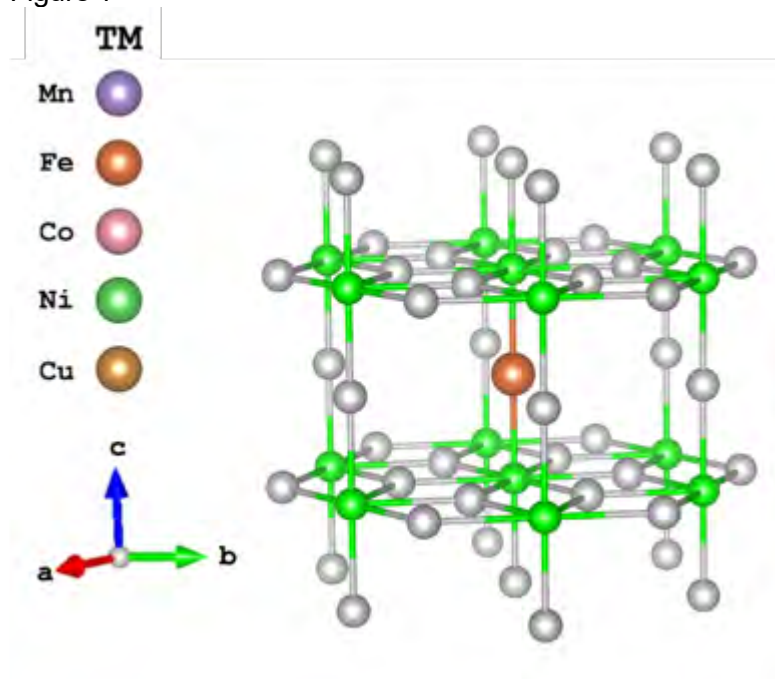


Figure 2

