From intermetallics to ion conductors

Luke Daniels – University of Liverpool

This seminar will summarise some examples of the latest research arising from the Rosseinsky group. We have recently discovered several intermetallic materials which adopt new derivatives of the NiAs structure type. Through substitution into materials such as NiBi and MnBi, it is possible to stabilise superstructures based on NiAs where the coupled formation of vacancies and filling of interstitial sites generate kagome nets within the transition metal layers. Such nets attract considerable attention due to the intrinsic topology introduced into the electronic band structure which can lead to unique phenomena and properties. In this family of "kagome-NiAs" materials, it is possible to obtain true hexagonal kagome motifs in non-polar materials such as $Ni_{0.7}Pd_{0.2}Bi$, or generate a net polarisation in materials such as $Ni_{0.79}Pd_{0.08}Bi$ through further vacancy ordering. We find these polar metals demonstrate unconventional electronic transport properties compared to the conventional metallic behaviour of the non-polar materials.

It is possible to demonstrate links between the structural chemistries of intermetallic materials and those of solid-state Li ion electrolyte materials through the identification of other types of structural nets. One well established example is the tetrahedral close packing of anions observed in argyrodite materials that reflects that of the metal packing in the intermetallic Laves phases such as $MgCu_2$. Laves phases, among other intermetallics, are well known to exhibit hydrogen uptake properties that can be related to ion conduction in ionic solids and may indicate an approach for designing new materials for Li ion conduction. The Rosseinsky group has studied a number of new materials as potential Li ion conductors in recent years, including oxide-halide argyrodites,[1] ultraphosphate compounds with extended condensed frameworks,[2] and sulphide-halide materials.[3] I will provide a summary of these alongside materials from the wider literature, discuss some thoughts on the impact of certain structural features and motifs on Li ion conduction, and the importance of being able to access them via particular chemistries, e.g. through the use of multiple anions.

Bio

Luke completed his PhD in materials chemistry at the University of Warwick in 2015, under the supervision of Professor Richard Walton and Dr Alex Hannon, focusing on the solution synthesis of new mixed metal oxides, making use of diffraction and total scattering methods to correlate structural disorder to their magnetic properties. Luke joined the group of Professor Matthew Rosseinsky FRS in 2016 as a PDRA and studied new oxide thermoelectric materials, specialising in the structural characterisation, processing and transport measurement of ceramics. He took up his current position of Research Coordinator at the University of Liverpool at the start of 2019 where he manages a portfolio of solid-state chemistry projects focused on the design and discovery of new materials aimed towards a wide range of potential applications. Luke's research interests involve developing an understanding of structure-property relationships in functional materials through a range of characterisation techniques.

[1] Morscher et al., J. Am. Chem. Soc., (2022) 144, 22178-22192.

[2] Han et al., *J. Am. Soc. Chem*., (2021) 143, 18216-18232.

[3] Vasylenko et al., Nat. Commun., (2021), 12, 5561