**Development of a synthesis route for YScS3, a potential sulfide p-type TCM**

E. N. Teather1,2, P. Komar3,4, D. Payne2, R. Perry1

*1 First author's affiliation, City, Country 1Department of Physics, University College London, London, UK*

 *2Department of Materials, Imperial College London, London, UK
3STFC, UK
4Department of Chemistry, Keele University, Keele, UK.*

Within novel transparent conducting materials (TCMs), developing a high-quality p-type remains elusive. Until recently, oxides have primarily been explored for TCMs, because their chemistry is well understood and they are affordable and relatively easy to synthesise. However, oxide p-types consistently show low conductivity[1]. This has been attributed to the high electronegativity of oxygen ‘trapping’ holes around the oxide ions, leading to a high hole effective mass. Other chalcogenide anions offer an alternative, having lower electronegativity while retaining similar bonding behaviour. This approach has seen some success, with reports of conductivities up to 1000 S cm-1 for sulfide TCMs, compared with approximately 400 S cm-1 for oxides[1]. However, these are not yet comparable to n-types, so further research is necessary. One challenge is that non-oxide materials can be difficult to synthesise, impeding their development.

In 2020 Zhang et al.[2] predicted Zn-doped YScS3 as a good p-type TCM, with a low calculated hole effective mass of 0.48 m0, comparable to the electron effective mass of ITO[3]. YScS3 has previously been synthesised[4], but its properties were not studied. We have developed new methods to synthesise YScS3. Powders have been synthesised by conversion of the oxides under CS2 gas, from which pure single crystals were grown by chemical vapour transport. Zn-doped powders have been synthesised in a two-step method, with Sc-deficient powders formed under CS2, followed by incorporation of Zn in a sealed tube. This will enable YScS3 to be assessed as a TCM. Moreover, optimizing the synthesis of YScS3 provides insights for producing other novel sulfide TCMs.

**References**

[1] S. K. Maurya et al., Energies, 15, 8698, 2022

[2] H. Zhang et al., Chinese Physics Letters, 37(9), 097201, 2020

[3] S. F. J. Blair et al., Nanomaterials, 13(13), Art. no. 13, 2023

[4] N. Rodier et al., Comptes rendus hebdomadaires des séances de l’Académie des sciences, Série C, 270, 2127, 1970