Contribution ID: **151** Type: **Oral Presentation**

Single crystal growth and physical properties of tetragonal $BaMn_2P_2$

Wednesday, 5 July 2023 14:40 (20 minutes)

The discovery of unconventional superconductivity (SC) in doped iron-based arsenide $BaFe_2As_2$ [1] crystallizing in $ThCr_2Si_2$-type structure ignited interest in 122 tetragonal systems. Substituting iron with other 3d or 4d transition metal ions that constitute the metal-pnictide sublattice in similar systems have yielded interesting results including, but not limited to, low-temperature SC [2], half-metallic behaviour [3], new layered magnetic phases [4] and highly frustrated itinerant magnetism [5]. The Mn based $BaMn_2Pn_2$ compounds [Pn = P, As, Sb, Bi] are small band gap semiconductors with stacked-square-lattice of Mn ions that order antiferromagnetically at temperatures higher than room temperature. Although As, Sb and Bi based compounds have been thoroughly investigated [6-9], the experimental work on $BaMn_2P_2$ is dated and limited [10,11]. In this contribution, we report the synthesis and growth of single crystals of $BaMn_2P_2$ as well as its structural, electronic, magnetic and thermal properties. Electrical resistivity and heat capacity measurements indicate that $BaMn_2P_2$ has an insulating ground state with a small band gap. Anisotropic magnetic susceptibility measurements show that similar to its As-, Sb- and Bi- counterparts, $BaMn_2P_2$ has collinear Néel type antiferromagnetism below T_N = 795(15) K, which is the highest value for 122- pnictide compounds reported so far. The magnetic susceptibility increases above T_N suggesting that antiferromagnetic correlations persist above the magnetic ordering temperature—a feature which was also observed in the As-, Sb- and Bi- based compounds. This can be explored further through hole-doping studies as in the case of $BaMn_2As_2$ with T_N = 618 K, which resulted in half-metallic behaviour with T_c = 100 K which is of significance as high T_c half-metals are ideal for spin-polarized transport-based applications. These results were recently published in Phys. Rev. Mater. **7**, 044410 (2023).

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Apply to be considered for a student ; award (Yes / No)?

No

Level for award;(Hons, MSc, PhD, N/A)?

N/A

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Session Classification: Physics of Condensed Matter and Materials Track 1

Track Classification: Track A - Physics of Condensed Matter and Materials