

# Understanding The Local Spin Structure of $\text{MnPS}_3$ and $\text{MnPSe}_3$ Through Magnetic Pair Distribution Function Analysis

Raju Baral<sup>1</sup>, Jue Liu<sup>1</sup>, Nan Huang<sup>2</sup>, David Mandrus<sup>2</sup>, Stuart Calder<sup>1</sup>

<sup>1</sup>*Oak Ridge National Laboratory*, <sup>2</sup>*University of Tennessee*

[baralr@ornl.gov](mailto:baralr@ornl.gov)

$\text{MnPSe}_3$  and  $\text{MnPS}_3$  are 2D van der Waals antiferromagnetic materials with respective Néel temperatures of 74 K and 78 K. Despite the similar ordering temperatures, the magnetic behavior is distinct, with out-of-plane spins in  $\text{MnPS}_3$ , but spins confined to the  $ab$ -plane for  $\text{MnPSe}_3$ . While both these materials exhibit stronger magnetic interactions in the  $ab$ -plane in comparison to the out-of-plane, the relative strength alter significantly. In our study we investigated the series  $\text{MnPS}_x\text{Se}_{3-x}$  via total neutron scattering measurements to gain insight into the local magnetic structure and local spin correlation in the paramagnetic region as well as in the ordered phase. We adopted magnetic pair distribution function (mPDF) analysis of the neutron data to understand the short-range magnetic correlations in these materials and how these magnetic correlations change as we introduce disorder on S/Se site in  $\text{MnPSe}_3$  and  $\text{MnPS}_3$ .