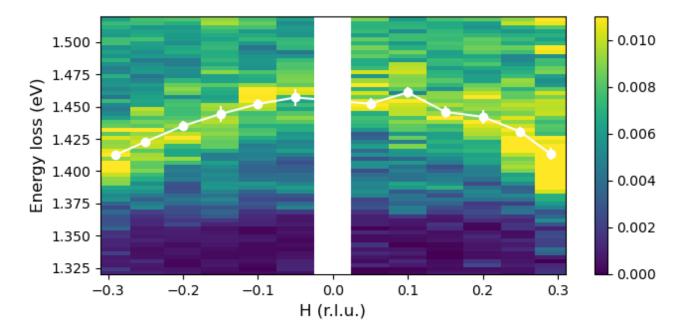
ESRF	Experiment title: Zhang-Rice Exciton propagation in van der Waals antiferromagnet NiPS3	Experiment number: HC-5030 Ref. #91753
Beamline:	Date of experiment:	Date of report:
ID32	from: September 13, 2022 to: September 19, 2022	February 23, 2023
Shifts:	Local contact(s):	Received at ESRF:
18	Flora Yakhou-Harris	
Names and affiliations of applicants (* indicates experimentalists):		
Mark Dean*		
Wei He*		
Yao Shen*		
Matteo Mitrano		
Krzysztof Wohlfeld		
Jennifer Sears		

Report:

During this beamtime we successfully collected RIXS measurements of the Zhang-Rice exciton in a single crystal of CrSBr. This material is a van der Waals antiferromagnet with conceptually similar physics to that of NiPS₃, the compound originally designated in the proposal. By agreement with ID32 Beamline Responsible we decided to change materials because others are working on this topic too and were concerned about the low chances of this data being able to be incorporated into a high impact publication.

Our measurements were successful in detecting the Zhang-Rice exciton, at energies just below the crystal field excitations. The q-dependent measurements along the reciprocal space H and K directions both show a dispersion of approximately 50 meV, of the same order of magnitude as the magnon dispersion. CrSBr is known to have a 1D electronic character, so the presence of two dimensional dispersion is suggestive of the magnetic character of this excitation. The data quality is sufficient to accurately extract peak positions, as demonstrated in the exciton dispersion in the H direction shown below:



We also characterized the temperature and polarization dependence to determine the interaction of the exciton with the magnetically ordered state, and the orbital composition of the exciton. We are confident that this data set will allow us to construct a comprehensive picture of the behaviour of the Zhang-Rice exciton in CrSBr. Data fitting and theoretical modelling is currently in progress, and we anticipate that the results result in a high impact publication.