



	<b>Experiment title:</b> Plasmon dispersion in layered transition-metal dichalcogenides	<b>Experiment number:</b> HC- 730
<b>Beamline:</b>	<b>Date of experiment:</b> from: 26 June 2013 to: 02 July 2013	<b>Date of report:</b> 13.10.2014
<b>Shifts:</b>	<b>Local contact(s):</b> Ali Al-Zein	<i>Received at ESRF:</i>
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## Report:

At the upgrade beamline ID20/UPBL6 (inelastic x-ray scattering), we measured the plasmon dispersion in transition metal dichalcogenides NbSe<sub>2</sub> and Cu<sub>x</sub>NbS<sub>2</sub>.

The results have been published in Cudazzo et al., *High-energy collective electronic excitations in layered transition-metal dichalcogenides*, Phys. Rev. B **90**, 125125 – Published 16 September 2014

## Abstract:

We characterize experimentally and theoretically the collective electronic excitations in two prototypical layered transition-metal dichalcogenides, NbSe<sub>2</sub> and Cu<sub>0.2</sub>NbS<sub>2</sub>. The energy- and momentum-dependent dynamical structure factor was measured by inelastic x-ray scattering (IXS) spectroscopy and simulated by time-dependent density-functional theory. We find good agreement between theory and experiment, provided that Nb semicore states are taken into account together with crystal local-field effects. Both materials have very similar spectra, characterized by two main plasmons at 9 and 23 eV, which we show to both have  $\pi+\sigma$  character on the basis of a detailed analysis of the band structure. Finally, we discuss the role of the layer anisotropy in the dispersion of these plasmons.