



	<b>Experiment title:</b> Plasmon dispersion in layered transition-metal dichalcogenides	<b>Experiment number:</b> HC-730
<b>Beamline:</b> ID20	<b>Date of experiment:</b> from: 26 June 2013 to: 02 July 2013	<b>Date of report:</b> 2/3/2015
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**Report:**

The results of this experiment have been published in

“High-energy collective electronic excitations in layered transition-metal dichalcogenides”

by Pierluigi Cudazzo, Kari O. Ruotsalainen, Christoph J. Sahle, Ali Al-Zein, Helmuth Berger, Efren Navarro-Moratalla, Simo Huotari, Matteo Gatti, and Angel Rubio: Physical Review B 90, 125125 (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 have both  $\mid + \leftarrow$  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.