By comparison of momentum-resolved electron energy-loss spectra and ab-initio calculations we analyze high-energy plasmons in 2D heterostructures made of graphene and few- or monolayer MoS₂.

We are particularly interested in MoS₂ monolayers covered by graphene (G/MoS₂/G sandwiches) as it has been shown that such a configuration protects the MoS₂ from beam damage [1].

Our experiments have been performed using a low-voltage (20–80 kV) transmission electron microscope with simultaneous acquisition of spectra for different momentum transfers. We have recorded energy-loss spectra in the range of 0–50 eV for momentum transfers along certain crystallographic axes within the Brillouin zone. For very high momentum and energy resolution, we have used a monochromated Zeiss Libra 200 based TEM in diffraction mode with an in-column Ω energy filter (SALVE II [2,3]).

The corresponding ab-initio calculations have been performed as follows: For the ground-state simulations, we have used the density-functional theory (DFT) software ABINIT [4] with pseudopotentials and local-density approximation (LDA). Energy-loss spectra have been calculated with the dp-code [5] within the random-phase approximation (RPA).

Eventually, deficiencies in both the experimental data and the simulations can be spotted by comparing the ab-initio calculations to the corresponding electron energy-loss spectra. These deficiencies include consequences of the approximations we made in the ab-initio calculations. Besides, our measurements are subject to the following experimental difficulties: First, despite the use of low acceleration voltages, the beam-sensitivity of the MoS₂ monolayers limits the acquisition times of the spectra. During an exposure of only a few minutes, beam damage and contamination may lead to significant changes in the spectra. Second, the signal decays drastically with increasing momentum transfer, so that the background noise of the CCD plays a crucial role.