Modelling Spatially-Resolved Electron Energy-Loss Spectra in the Low-Loss Region

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Mapping low-energy excitations such as plasmons, excitons, or phonons with high spatial and spectral detail is key for understanding and engineering nanostructured materials' optical, electrical, or thermal properties. One of the experimental techniques allowing for analyzing the low-energy excitations and their interaction down to the atomic scale is electron energy-loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM), which enables the acquisition of spectra with a few-meV/Å spectral/spatial resolution [1,2].

Most of the recent state-of-the-art STEM-EELS experiments have been complemented or even guided by theoretical modelling and predictions. This talk will review two main approaches for simulating low-loss EEL spectra, using either classical electrodynamics or ab-initio methods. I will show that the macroscopic electrodynamics calculations are suitable for describing polaritonic excitations, such as plasmon or phonon polaritons that typically emerge in metals or ionic crystals, respectively. I will discuss examples of spatially-resolved EELS of electron-beam excitation of phonon polaritons in hexagonal boron nitride [3] and a system sustaining plasmon and phonon polaritons, which are engineered to strongly couple [4].

On the other hand, STEM-EELS of molecular systems or momentum-resolved EELS requires modelling at a truly microscopic level, which I will demonstrate with an example of a hBN-like molecule. The theoretically predicted results obtained with ab-initio calculations demonstrate that a single isotope impurity in this molecule would significantly affect the EELS probability [5]. Finally, we will discuss possible future directions in STEM-EELS, considering both theoretical and experimental efforts.

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