

Supplementary material: DFT modeling of low-loss EELS in wurtzite III-nitride ternary alloys.

Alberto Eljarrat^{1,*}, Xavier Sastre¹, F. Peiró¹, and S. Estradé¹

¹Laboratory of Electron NanoScopies, LENS-MIND-IN2UB, Dept.

Electrónica, Universitat de Barcelona, Martí i Franqués 1, 08028

Barcelona, Spain

References

- [1] EELS data-base web: <http://eelldb.eu>. Spectra submitted by M. Cheynet Laboratory of Thermodynamics and Metallurgical Physics and Chemistry (LTPCM), Grenoble (France)

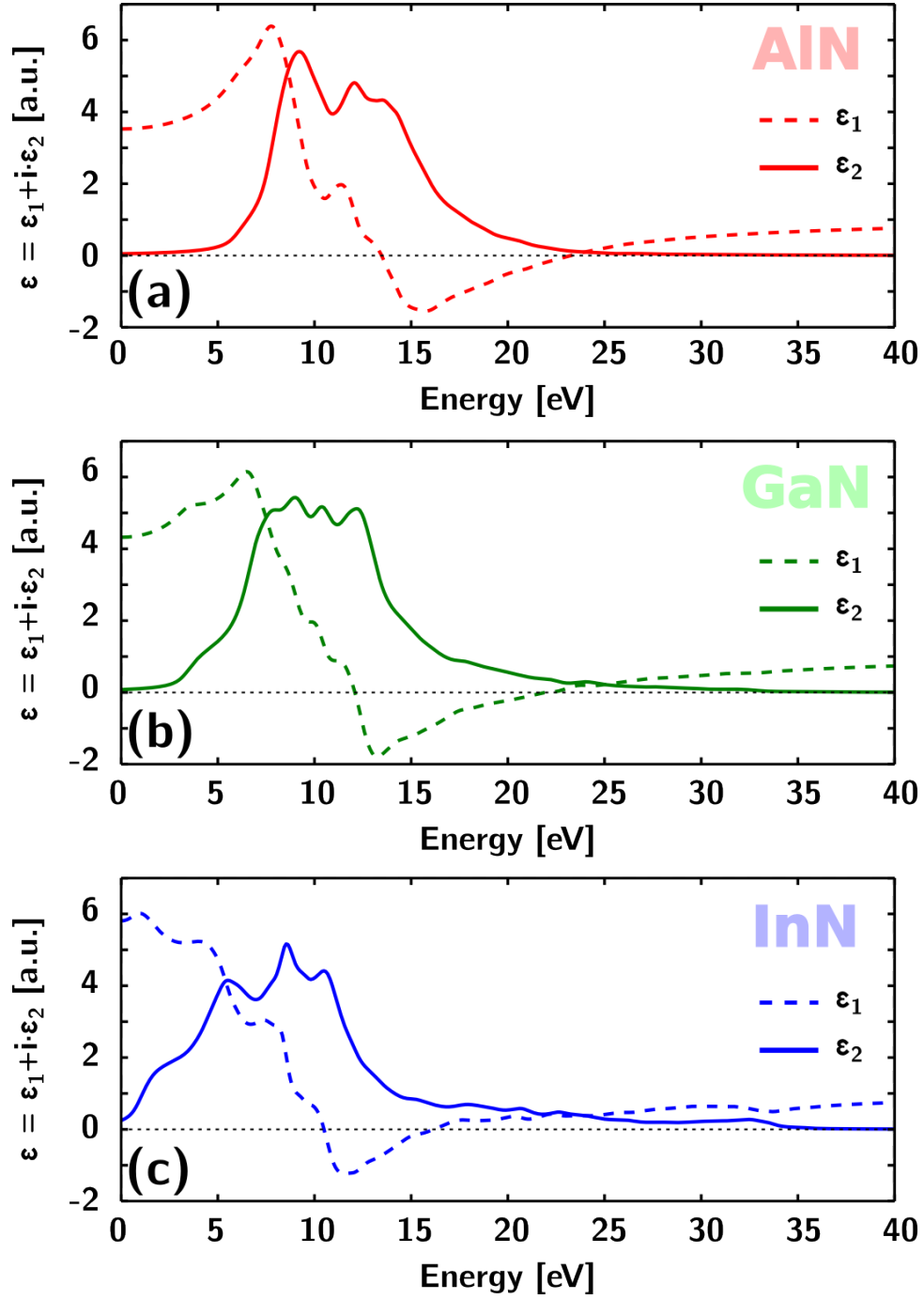


Figure S1: From top to bottom: the complex dielectric functions (CDF) from the three binary materials, AlN, GaN and InN. Real and imaginary parts are depicted using dashed and solid lines, respectively.

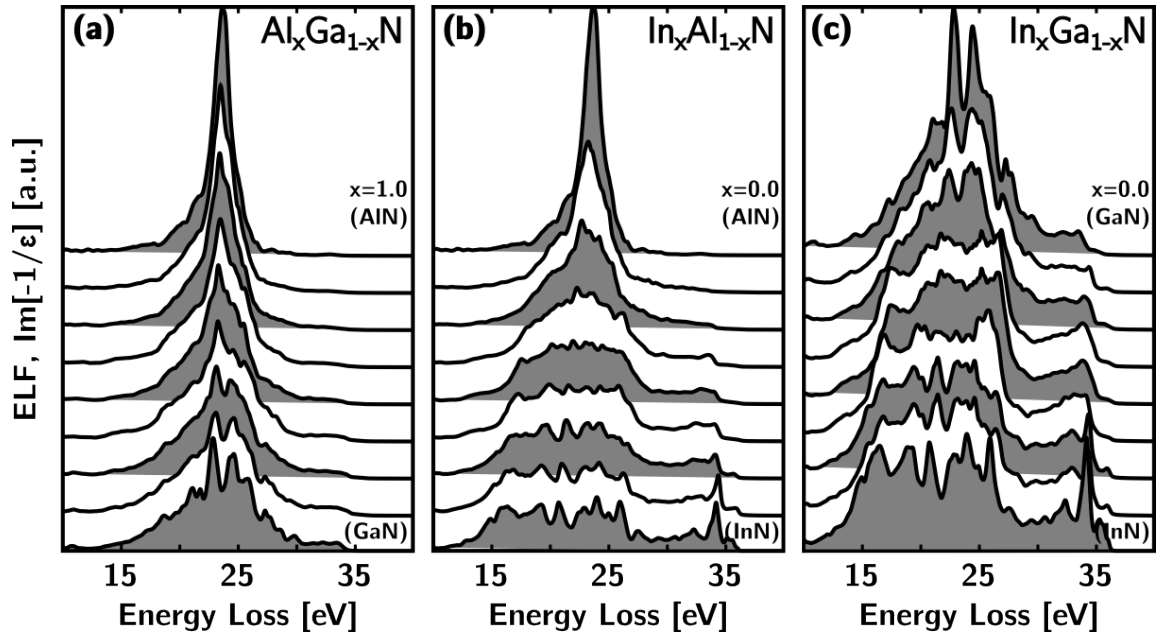


Figure S2: The obtained energy-loss function (ELF) series after the simulation of the three ternary compounds, $\text{Al}_x\text{Ga}_{1-x}\text{N}$, $\text{In}_x\text{Al}_{1-x}\text{N}$ and $\text{In}_x\text{Ga}_{1-x}\text{N}$. The ELF-series correspond to 0.1 broadening, showing unrealistically sharp peaks in the spectra. These ELF-series are depicted as in Fig. 4 in the main document.

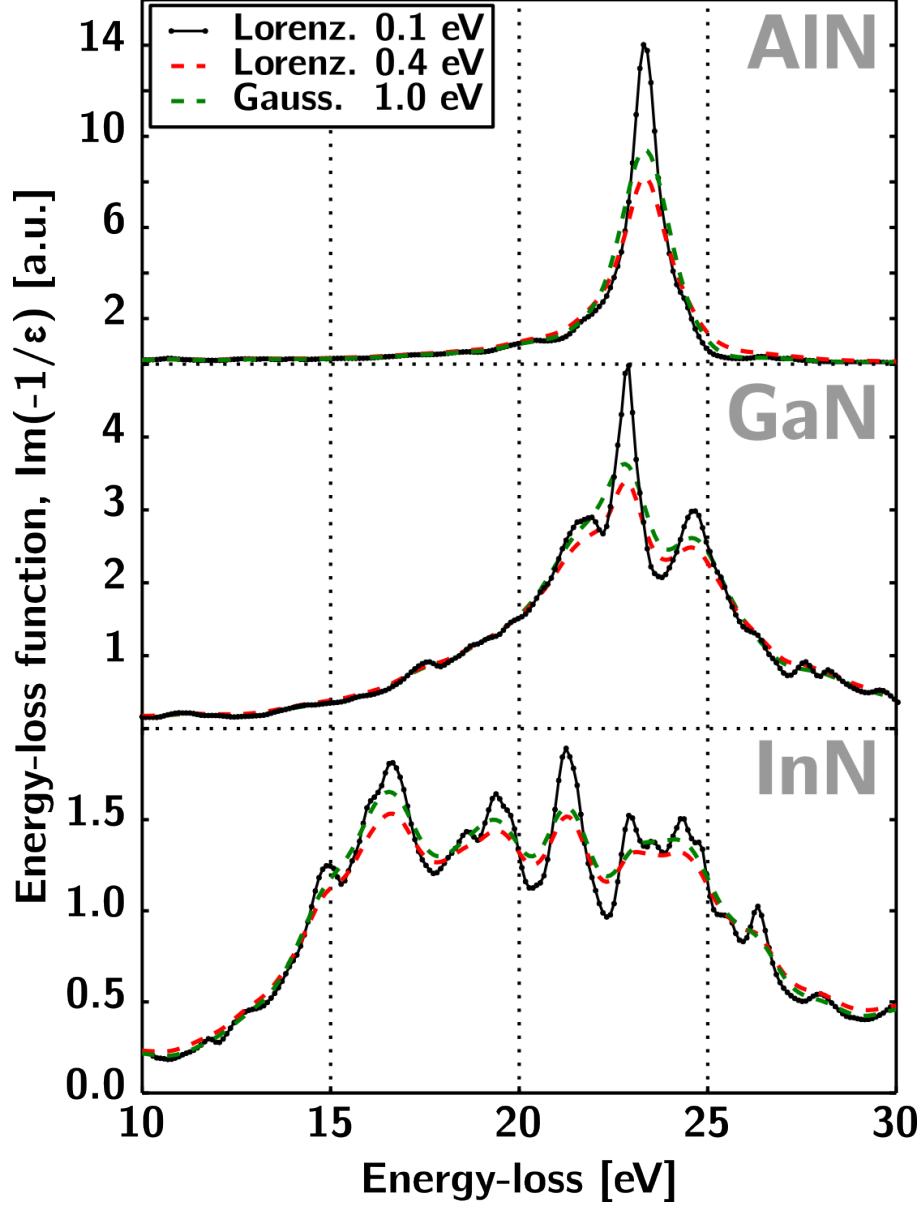


Figure S3: From top to bottom, comparison between different broadenings applied to the calculated ELF of AlN, GaN and InN, respectively. Lorentzian broadening with $\Gamma = 0.1$ eV is depicted using black solid lines and point-markers. Lorentzian broadening with $\Gamma = 0.4$ eV (as used in this work) is depicted using dashed green lines. Gaussian broadening with $\Gamma = 1.0$ eV is depicted using dashed green lines.

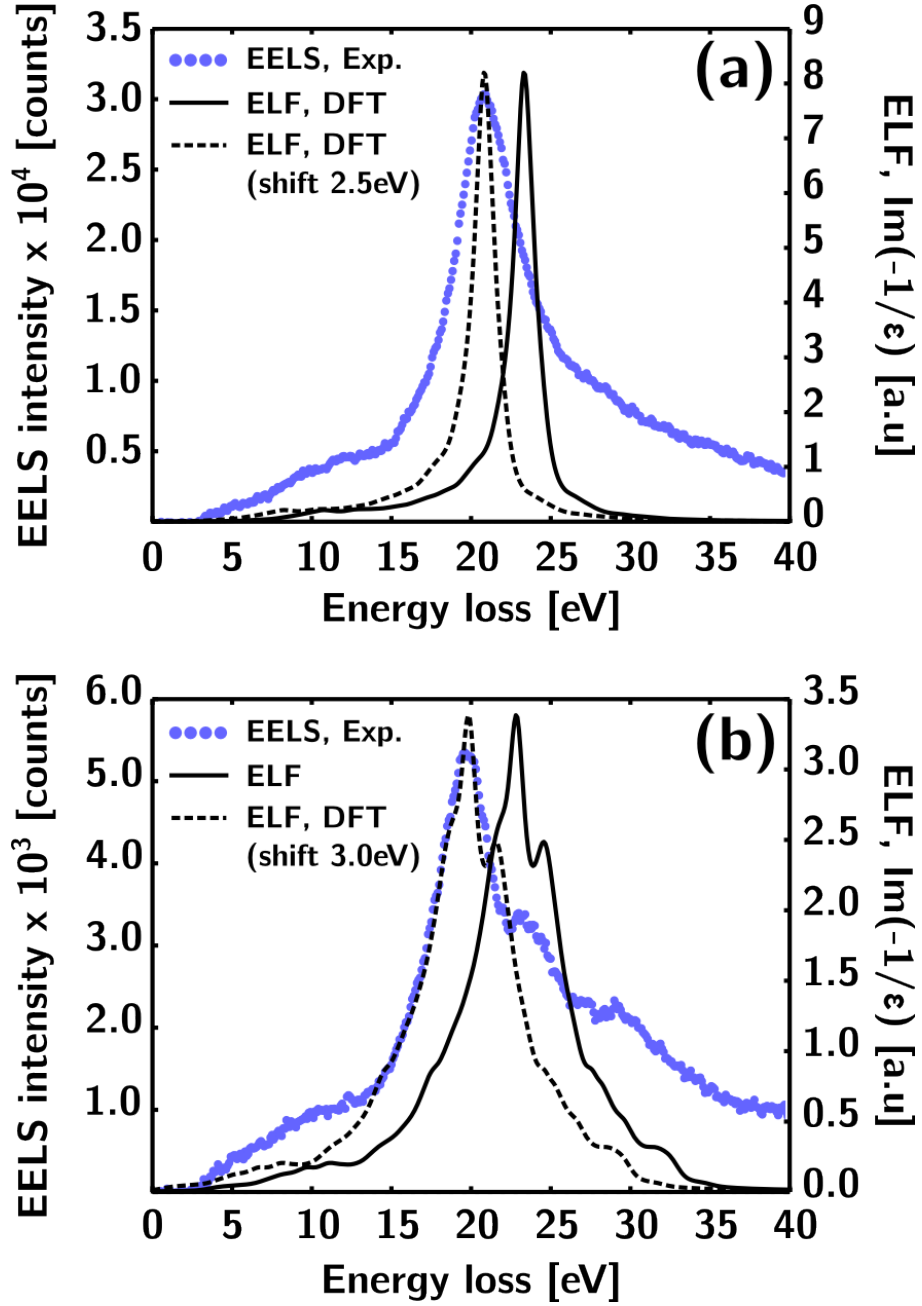


Figure S4: From top to bottom, comparison between the simulated ELF (lines) and experimental EELS (dots) for AlN and GaN, respectively. A shifted version of the ELF, dashed lines, is included to help visual examination as the obtained ELF show higher plasmon peak energy than the experimental EELS. Experimental data obtained from the EELS data-base (See Ref. 1). InN has not been included in this figure as experimental EELS data for this material was not available at the time of preparing this work.