First-Principles Approach for Spatially-Resolved Electron Energy-Loss Spectroscopy

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The combination of electron energy-loss measurements (EELS) with corresponding *ab-initio* calculations has been very productive for the study of collective electronic excitations (plasmons) in solids and nano objects. While most of these investigations have been angular resolved, recent advances in electron microscopy allow for spatial resolution down to the atomic level and call for corresponding theoretical investigations.

We present a first principles approach for spatially resolved EELS for valence losses (less than 40 eV), which we applied to Carbon systems: Within the framework of density functional theory, we calculate the ground state of the system with the ABINIT code [1]. The loss of the impinging electron is then computed in first order perturbation theory, explicitly taking into account the inhomogeneity of the system on the atomic level [2].

Additionally, our *ab-initio* calculations give access to the spatial distribution of collective electronic oscillations in a system that is subject to an external perturbation (see Figure 1).

1. ABINIT-code: http://www.abinit.org
2. DP-code: http://www.dp-code.org; V.Olevano et.al., unpublished.

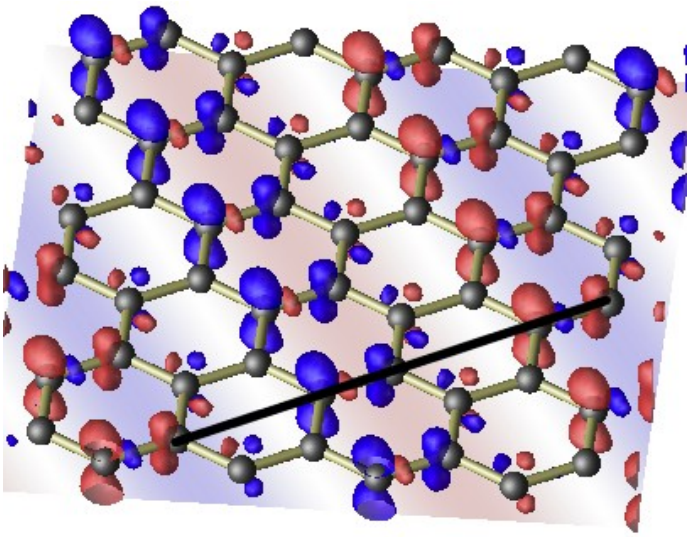

Figure 1. Calculated charge density oscillation in graphite due to an external plane wave perturbation with energy ħω=9eV and an in-plane momentum q=0.74Å-1 (the black line indicates the corresponding wavelength). The red (blue) isosurface correspond to a decreased (increased) electron density which corresponds to a polarization of the π-electrons.

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