Simulating advanced excitation energy loss spectroscopies of molecular excitations

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Electron energy loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM) is becoming an important technique in spatially resolved spectral characterization of optical and vibrational properties of matter at the nanoscale [1]. Very recently, a new device composed by nanoscale holograms [2,3] or electrostatic phase elements allows analyzing the single components of orbital angular momentum (OAM) by spatially separating them (Fig. 1, top). Such an OAM-sorter drastically enhances EELS as innovative double-dispersed spectroscopy experiments.

In this work [4], we modified the theoretical framework needed to describe conventional low-loss EELS experiments in STEM, introducing a TD-DFT description of the molecular systems. Our work paves the way to study electronic transitions in single chromophores or supramolecular aggregates and devise new experiments [4,5] for the analysis of these excitations (Fig. 1, bottom).

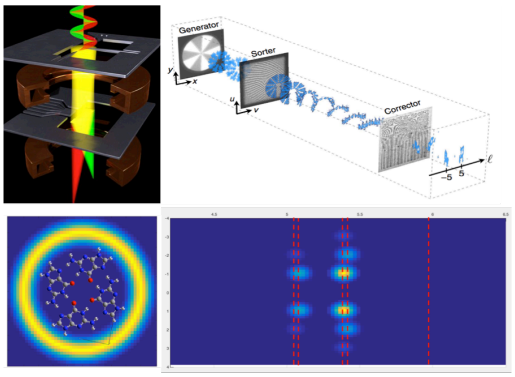

Figure 1: Top: scheme of the experimental apparatus of an electron beam carrying OAM. Bottom: TD-DFT simulation of OAM-resolved EELS experiment on a guanine-tetramer.

References

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