Optical spectra of strained carbon nanotubes: *Ab initio* predictions

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CNTs show unique properties upon strain: Under load, their band gap is opening or closing (depending on the CNTs' chirality) which makes them suitable for electronic and optical strain sensing at the nano scale. Further, they could operate as strain-tunable emitters.

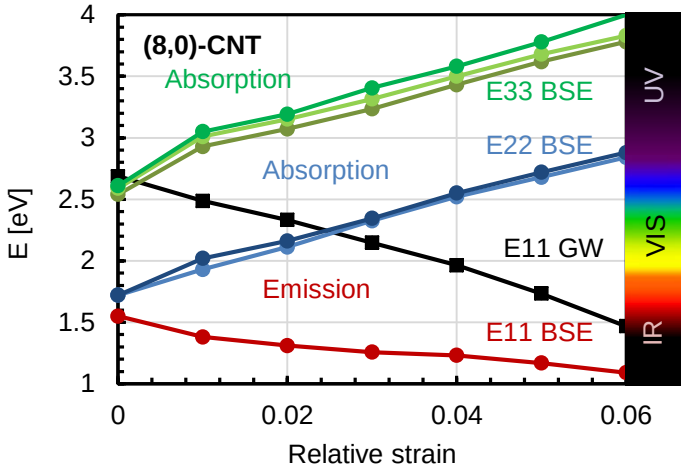

Fig.1: Optical transitions of an (8,0)-CNT on strain.

Our theoretical investigations of strained CNTs show strongly bound excitons that drastically modify the optical spectrum of CNTs with respect to single-particle pictures. The resulting optical transitions strongly shift with respect to strain. However, the shift of the optical transition differs from the shift of the corresponding electronic state. Additionally, the strain-dependent, intrinsic carrier screening alters the exciton binding energy.

Higher optical transitions, depending on their order, shift either in the same or in the opposite direction compared to the first one. This behavior originates from the shift of the electronic bands, which can be qualitatively understood by the tight-binding zone folding scheme. Quantitatively, the exciton binding strength is a function of the band gap and changes on strain. One exemplary result is that the second optical transition of the (8,0)-CNT shifts through the whole visible spectral range if strained up to 5% (see fig. 1).

For our calculations, we use independent-particle (density functional theory, DFT) and single-quasiparticle band structures (G0W0@LDA) to investigate the strain-dependence of the band gap. Further, the Bethe-Salpeter equation is applied for the calculation of the optical spectra in order to describe excitonic effects. In a one-dimensional system, these calculations require the truncations of the Coulomb interaction between periodic images in the supercell approach.

The parameters obtained by these calculations can be used for optical device modeling based on strained CNTs as well as CNT spectroscopy, e.g. infrared spectroscopy, and may allow an extrapolation to other CNTs.

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