Redshift of excitons in carbon nanotubes caused by the environment polarizability: A BSE study

MICHAEL ROHLFING, University of Osnabrueck, Germany — Optical excitations of molecular systems can be modified by their physical environment. We analyze the underlying mechanisms within many-body perturbation theory (GW approximation and Bethe-Salpeter equation, BSE), which is particularly suited to study non-local polarizability effects on the electronic structure. Here we focus on the example of a semiconducting carbon nanotube, which observes redshifts of its excitons when the tube is touched by another nanotube or other physisorbates. We show that the redshifts mostly result from the polarizability of the attached ad-system. Electronic coupling may enhance the redshifts, but depends very sensitively on the structural details of the contact.