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Optical Properties of Nano-Crystallites¹

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The optical properties of nanostructured materials are interesting due to the tunability of the electronic structure, of the lifetimes, and of the excitation spectra. This calls for precise knowledge of the physical effects which create the desired properties. Thereby it is of utmost importance to settle the question as to how many-body effects have to be incorporated in the description of the excitation aspects inherent in any optical process.

Static DFT-LDA *ab initio* calculations have now become possible for systems of about 1000 atoms for the ground state. Time-dependent DFT (TDDFT) can in principle describe excitations as exhibited in optical spectra. However, approximations for the exchange and correlation contributions that are valid in a wide range of situations and efficient enough to be applied to large nanostructures are still to be found. GW calculations deal only with charged (electron addition and removal) excitations. The solution of the Bethe-Salpeter equation (BSE) gives good answers for neutral excitations like absorption but is numerically heavy and so far tractable for rather small systems only.

In my talk I will briefly review the state of the calculation of optical properties. Using bulk semiconductors and Ge, Si, and alloy nanocrystals as illustrations, I will then discuss the following points:

- Manifestation of confinement effects in various spectra;
- Importance of surface effects;
- Interplay between many-body effects and confinement and surface effects;
- Importance of short- and long-range contributions. How are they adequately described? (Important, e.g., for embedded nanostructures.)

These questions will be discussed in view of the optical properties, but also for loss spectra and photo-emission. Methods used are DFT-LDA, TDDFT in various approximations, GW, and BSE.

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