Optical activity spectra of carbon nanostructures via a novel π-electron model

Péter R. Nagy [1], Péter R. Surján[1] , Ágnes Szabados[1]

[1] Laboratory of Theoretical Chemistry, Eötvös University, Hungary

E-mail: nape@coulson.chem.elte.hu

Characterization of chiral carbon nanostructure samples, such as fullerenes and carbon nanotubes are still a challenging task, since the spectroscopical tools are limited to electronical and vibrational optical activity (OA).

To interpret the OA spectra of these systems quantum chemical methods are necessary. Due to large system size, we choose a cost-effective, one-particle π-electron method. Our studies focus on spectral line intensities of inelastic light scattering, i.e. Raman and vibrational Raman Optical Activity (VROA).

We find that π-electron methods, relying on the first neighbour approximation (Hückel-model) describe the Raman spectra of fullerenes well, but one has to include one-particle integrals between all sites to obtain reliable VROA spectra.

Parameters of the π-model are derived from ab initio calculations in a system-specific manner, in the spirit of the Bloch-equation. Standard linear response theory is used to calculate spectral intensities.