Photoluminescence of Undoped Cis- Polyacetylene Semiconductor Material

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Abstract

Photoluminescence (PL) is one of the key experimental characterizations of optoelectronic materials, including conjugated polymers (CPs). In this research, we selected a simplified model of undoped cis-polyacetylene (cis-PA) oligomer which is used to explain the mechanism of photoluminescence (PL) [1] of the CPs. Using the combination of ab initio electronic structure and time-dependent density matrix methodology, the photo-induced time-dependent excited state dynamics were computed. We explore the phonon-induced relaxation of the photo-excited state for a single oligomer of cis-PA. Here, the dissipative Redfield equation of motion [2-4] of the motion is used to compute the dissipative excited state dynamics of electronic degrees of freedom. This equation uses the nonadiabatic couplings as parameters. The computed excited state dynamics shows that the relaxation rate of the electron is faster than the relaxation rate of the hole. The dissipative excited-state dynamics are combined with radiative recombination channels to predict the PL spectrum [1]. Our simulated results show that the absorption and emission spectra both have a similar transition. The main result is that the computed PL spectrum demonstrates two mechanisms of light emission originating from (i) the inter-band transitions, corresponding to the same range of transition energies as the absorption spectrum and (ii) intra-band transitions not available in the absorption spectra.

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