

Electronic properties of polymethine systems 9: position of soliton level in charged molecules

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<https://doi.org/10.1016/j.dyepig.2004.06.019>

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Abstract

The disposition of electron levels in the cations and anions of linear conjugated systems is considered as compared with the pattern neutral molecules. It is found that the injection or removing of an electron causes the so-called “soliton level” to appear in the energy gap and the valence band top and conduction band bottom are shifted considerably up with anions and down with cations, due to the electron–electron interaction in the charged π -systems. The influence of the terminal donor and acceptor groups on both the position of the soliton level and band is modeled by $-\text{NH}_2$ and $-\text{CH}=\text{O}$ residues; it is shown that the energetic effect of the donor group is greater in cations while anions are more sensitive to the acceptor groups.
