

Soliton dynamics and impurities in the Pariser-Parr-Pople model of alternating trans-polyacetylene. Markus, R.; Foerner, W.; Ladik, J

Abstract

The influence of site and bond impurities on soliton dynamics in alternating trans-polyacetylene using the PPP model is studied by continuously changing the corresponding parameters. For both site and bond impurities, soliton movement is possible only within a small range of parameter changes caused by the impurities. For the carbon-carbon resonance integral only within a small interval around the Huckel value of 2.5 eV was a moving soliton found.