Soliton dynamics in a formamide stack using a Taylor-series expansion for the potential surface. II. The Pariser-Parr-Pople Hamiltonian. Foerner, Wolfgang; Ladik, Janos; Otto, Peter; Martino, Frank

Abstract

The effects of explicit electron-electron interactions described by the semiempirical PPP Hamiltonian on soliton dynamics in formamide stacks as a DNA model system are investigated. Explicit treatment of electron-electron interactions does not influence the properties of solitary waves in the model system. Possibilities that solitary waves might serve as charge carriers in stacked systems after doping are discussed.