

Conformational solitons in stacked systems. Hofmann, D.; Foerner, W.; Ladik, J

Abstract

With the help of numerical simulations using an extended Su-Schrieffer-Heeger-type Hamiltonian, the existence of solitary waves in a polyformamide stack is shown. A formamide dimer stack was chosen as a simplified model for the stacked nucleotide bases in DNA. Each formamide unit in the stack has 3 geometrical degrees of freedom during the time simulation. The passing of a solitary wave through the stack and its reflection at the end of the chain is shown. In addn., the collision of 2 solitary waves is discussed.