

Model calculation of the effect of hydration on the energy band structure of a nucleotide base stack. Otto, P.; Ladik, J.; Corongiu, G.; Suhai, S.; Foerner, W

Abstract

The energy band structure of the nucleotide base stacks poly(dC), poly(dT), poly(dA), and poly(dG) were calcd. by the ab initio SCF-LCAO crystal orbital method. For poly(dC), model calcns. were performed to investigate the effect of water mols. on its electronic structure. The presence of water mols., whose positions were previously detd. by a Monte Carlo simulation technique at 300 K, causes significant band shifts and, together with pos. ions, could substantially influence the conductive properties of native DNA.