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 calculated by the ab initio SCF-LCAO crystal orbital method. For poly(dC), model calculations were performed to investigate the effect of water molecules on its electronic structure. The presence of water molecules, whose positions were previously determined by a Monte Carlo simulation technique at 300 K, causes significant band shifts and, together with positive ions, could substantially influence the conductive properties of native DNA.