The energy band structure of polyfluoroethylene: influence of chemical substitution and conformation. Otto, P.; Ladik, J.; Foerner, W

Abstract

Ab initio SCF LCAO crystal orbital band structure calcns. for 6 different poly(fluoroethylene)s derived from trans-polyethylene replacing stepwise the H atoms by F atoms and for 18 helical configurations of PTFE [9002-84-0] are reported. The dependence of energy band structure on the basis set has been investigated. The theor. d. of electronic-state spectra is discussed and compared with the exptl. ESCA spectrum of PTFE, showing good agreement. The potential energy surface as a function of the rotation angle about the C-C bond agrees well with exptl. data.