Correlation-corrected energy bands of polymers with large unit cell: poly(para-phenylene) and poly(peri-naphthalene). Bogar, F.; Forner, W.; Kapuy, E.; Ladik, J

Abstract

The correlation-cor. band structures of quasi 1D poly(para-phenylene) (PPP) and poly(perinaphthalene) (PPN) are presented, using the ab initio quasi-particle method based on the iterative soln. of the inverse Dyson equation. A double zeta basis set is used with polarization functions for PPN and a double zeta basis is used for PPP.