Fourier Space Restricted Hartree-Fock Method For One-Dimensionally Periodic Systems.

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A method for the computation of the electronic structure of stereoregular polymers is reviewed. Its formulation makes use of the Fourier representation technique combined with the Ewald procedure for accelerating the convergence of lattice sums. This method is incorporated in the authors FT-1D program. This program exploits the spatial (line-group) symmetry (including rotational and screw axes, reflection and glide planes) in order to improve the efficiency of computation, extending to one-dimensional periodic systems the technique of Dupuis and King for building a complete Fock matrix from a minimal set of its matrix elements. Recently, the method has been extended to the computation of the electric polarizability at an "uncoupled" Hartree-Fock level of approximation, *i.e.* using Hartree-Fock wave functions and energies in the second-order perturbation theory polarizability expression, following the procedure of Blount and of Genkin and Mednis, as applied to polymers by Barbier, Delhalle, and André.

The features of this program are validated by reexamining the band structures of polyethylene, polysilane, and polytetrafluoroethylene. The results are consistent with previous works on the same systems, but exhibit better computational efficiency and greater achievable accuracy. Then, the performance of this method is illustrated for a problem of significant size: A single-wall (7,0) carbon nanotube with 56 spatial symmetry operations and with atomic basis sets containing up to 420 atomic orbitals per unit cell.

Ref: J.G. Fripiat, B. Champagne, and F.E. Harris, in J.R. Sabin, R. Cabrera-Trujillo, Eds; Advances in Quantum Chemistry vol. **71**, Elsevier : Amsterdam, 2015; pp 153-194 (2015).

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