

INTRODUCTION

ABSTRACT

This dissertation deals with the study of the electronic structure of a periodically-disordered polyethylene chain. The disordering is effected by the application of random rotations about consecutive C-C bonds, and the method of generation of the atomic coordinates is fully described.

The band structures of both the periodic and periodically-disordered chains are calculated using the extended Hückel method and the density of states derived therefrom.

The outstanding features of the band structure and the density of states of the aperiodic case are discussed via a comparison with the results of the periodic case. We then try to explain the significance of the outstanding features by considering a few theoretical expectations.

Finally, a plan for future work is outlined.