1. Abstract

Organic electronics are gaining a rapidly increasing share in the electronics industry, attracting scientists and researchers interest over the last few years. Organic materials combine low cost, ease of production and remarkable electronic and optical properties such as transparency, flexibility and the ability of tailoring theirs properties. The scope of this work is the theoretical investigation of the electronic properties of organic semiconducting materials such as acenes and rubrene.

First principle quantum mechanical calculations were performed based on the density functional theory (DFT) with the use of pseudopotentials in order to describe the ionic potential. Plane waves were used as a basis for the wave-functions. Exchange and the correlation terms between electrons were described using the local density approximation (LDA). A brief introduction to grid computing is given followed by results of a benchmark use of the ABINIT code installed on a grid computer to show the proper installation, function and abilities of the code.

Structural properties of acenes molecules (from benzene to pentacene) and rubrene is studied in order to get the stablest structure. The band structure and the Density of states (DOS) of acenes is computed and analysed to determine the band gap and bandwidth of each structure. Also known polymorphs of the pentacene molecule are studied to investigate the structural impact on the electronic properties. The relation between the structure of acene and band gap is shown, which is in agreement with previous studies, although band gap is underestimated systematically due to the known limitations of DFT-LDA method.

The conclusions of this work among with some discussion on the results and possible future work topics are include in the last chapter.