

A comparison of semiempirical and ab initio methods for calculating the electronic structure of C60 and C70 fullerenes

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The aim of this work is to find a method suitable at least for obtaining the isolated molecule band structure approximated by a Gaussian broadening of the discrete eigenvalues, to apply it for a first scan of bigger and more complex structures. We compared the results of several semiempirical and ab initio quantum-chemical methods to calculate the band structure of isolated C60 and C70 fullerenes. Theoretical results were compared with experimental photoemission and inverse photoemission spectra. The results show that Extended Hückel Theory is the best method of all analyzed here. It compares well with experimental results related to valence and conduction bands for fullerene but underestimates the valence-conduction band gap by about 50%. Therefore, it is suitable for a first screening of fullerene-like molecules. Finally, EHT is employed to predict the electronic structure of several hypothetical molecules (P60O60, N70, C30N30 and N60).