

## Electronic structure of organic semiconductors

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Organic semiconductors are among the most popular research objects in modern physics of semiconductors. Nanostructures based on organic materials are of great interest as materials for photo- and microelectronics. Effectiveness of their application requires an ability to understand and control of their electronic properties, such as ionization potential in solid and gase phase and quasiparticle energy spectrum. Widely used DFT method, which proved success in description of structural properties for many materials, fails in describing electronic spectrum, yielding qualitatively wrong results, such as greatly underestimated band gap in semiconductors. Hybrid density functionals (HF) provides simple way to roughly describe some many-electron effects and gives electronic spectra which agree well with photoemission results. However, this method still underestimates band gap. The HOMO-LUMO gap can be calculated by varying number of electrons in molecule as

$$\begin{aligned} E_g &= E_s^{LUMO} - E_s^{HOMO} = [E_{tot}(N+1) - E_{tot}(N)] - \\ &- [E_{tot}(N) - E_{tot}(N-1)] = \\ &= E_{tot}(N+1) + E_{tot}(N-1) - 2E_{tot}(N) \end{aligned}$$

In our research we are using HF for calculating electron spectra in valence and conductivity band for transition metal phthalocyanines, aromatic hydrocarbons, PTCDA. Our results spectra agree fairly well with available data of photoemission experiments[1]. Band gap calculated via energy difference is in excellent agreement with experimental data [2] and practically not affected by choice of density functional.

1. Navit Dori *et al.*, Phys. Rev. B **73**, 195208 (2006).
2. S.L. Murov, I. Carmichael *et al.*, *Handbook of Photochemistry* - M. Dekker, New York (1993).