

Silicon-organic pigment material hybrids for photovoltaic application

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Summary

We are running a project that is focussed on the development of silicon-organic pigment hybrid materials for thin film solar cell application. High conversion efficiency is expected from the combination of the advantages of organic dyes for light absorption and of silicon for charge carrier separation and transport. The project team, wants to find suitable dyes and deposition conditions for the preparation of photovoltaic hybrid materials. The functional composite materials will be prepared by (remote) hot wire chemical vapour deposition of silicon and co-sublimation of organic dye molecules. Dye molecules are synthesized and specifically modified in the group of our project partner D. Wöhrle (Uni-Bremen). The project team is completed by the group of D. Schlettwein (Uni-Oldenburg) with expertise on polymer based solar cells, and the group of M. Kunst (HMI-Berlin) with expertise on microcrystalline Si deposition and measurement of charge kinetics by time resolved microwave reflectivity.

The basic idea of the concept of bulk hybrid silicon-organic materials is displayed in Fig.1. Fig.1a shows a possible cell configuration with the silicon-organic composite sandwiched between highly n and p doped Si layers in a p-i-n structure. Fig.1b shows the band structure with the wanted energetic position of the dye HOMO and LUMO states just below the valence band maximum respective just above the conduction band minimum. Thereby injection of both, the photo-generated electron and hole into Si bands is energetically favoured and charge separation and transport occur in the Si-matrix. Increased absorptivity of the absorber layer, allows for a reduction of the film thickness.

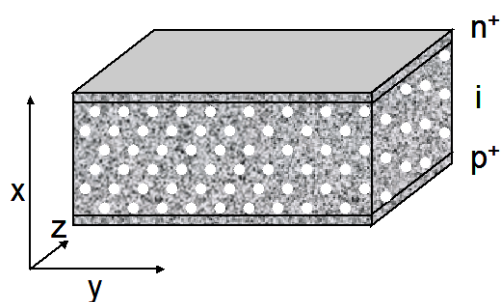


Fig.1a: Si-organic dye composite absorber in p-i-n structure.

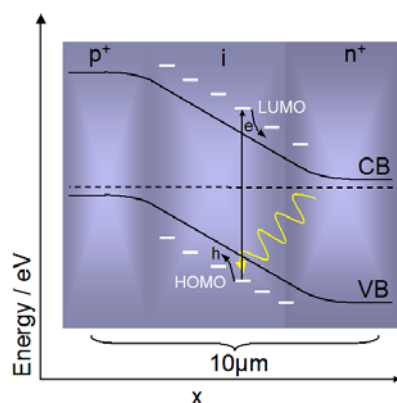


Fig.1b: Band structure with the wanted position of HOMO and LUMO states of the dye.

Stable organic pigments of high absorptivity are e.g. Metal-Phtalozyanines with molecular structure as displayed in Fig. 2a. While changing the central metal atom has little influence on position and width of the HOMO-LUMO gap, substitution of the ligand R shifts the gap without changing the width. Fig. 2b shows calculations (1) of HOMO-LUMO positions for Zn-

Phtalocyanines with R = H, and substituted by Cl or F. The width of the gap may be modified by changing the arrangement and number of carbon rings as e.g. in Tetraphenylporphyrin or Naphthalocyanine.

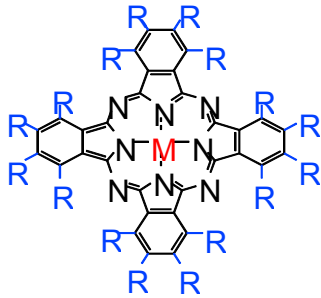


Fig.2a: Molecular structure of Metal- Phtalocyanines.

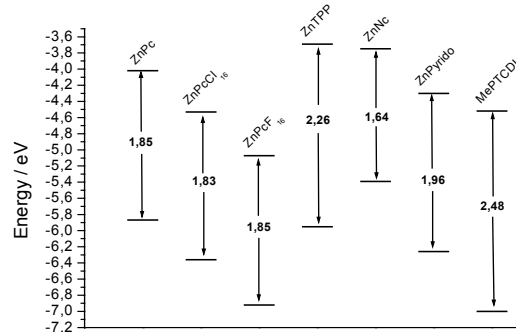


Fig.2b: Calculated HOMO-LUMO positions of different organic dye molecules.

Using UPS and SXPS we have measured the HOMO line up of ZnPc, substituted ZnPcF16 and ZnTPP on H-terminated Si (111) as displayed in Fig.3. In addition the position of the (adiabatic) HOMO-LUMO gap as measured with photoemission and inverse photoemission (2), the transport gap (relaxed charged molecule) and the optical (exzitic) gap are displayed where the values for relaxation and exziton binding energy have been taken as determined for CuPc (3) and in lack of experimental data equal values for relaxation energies of hole and electron are taken.

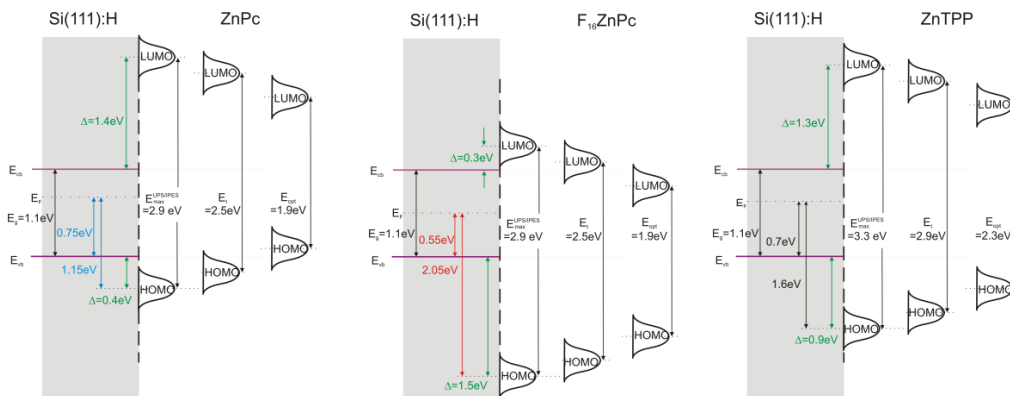


Fig.3: Alignment of dye HOMO-LUMO gap on Si:H. Indicated are the adiabatic, the (relaxed) transport gap and the optical (exzitic) gap.

The experimental determined shift of the HOMO-LUMO gap by F-substitution is very similar to the theoretical value. Injection of generated electron-hole pares from ZnTPP to Si should be favoured. For ZnPc injection of holes and for ZnPcF16 injection of electrons may be slightly hindered. Intermediate ZnPcCl16 should allow injection of electron-hole pairs.

- (1) G. Schnurpfeil, D. Wöhrle, unpublished results.
- (2) T.Schwieger, M. Knupfer, W. Gao, and A. Kahn Appl. Phys. Lett 500 (2003)
- (3) I.G. Hill, A. Kahn et al. Chem. Phys. Lett 327 (200)

