Thoughts about optimum materials and solar cell structures for the future.

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Photovoltaics is expected to supply electrical energy worldwide on a multi-terawatt scale. For Even though silicon or III-V compound cells are already well developed and reach efficiencies close to the theoretical maximum, ongoing developments could further contribute to the implementation of this important source of energy. Besides the exploration of suitable materials, novel device structures promise high efficiencies or significant economic advantages[i]. These developments are critically evaluated in view of feasibility and potential. The results are compared with the status of present technologies.

The basic concept of solar cell is well described by P. Wuerfel [ii]. The light absorbing part of the device is enclosed by membranes for the collection of holes and electrons respectively. The potential is created by the none-equilibrium of charge carriers. For efficient solar cell operation lifetime and transport of carriers in connection with selective contacts for electrons and holes are essential. Design criteria for solar cells should consider material properties and electronic structures compatible this solar cell principle.

Solar cell efficiencies close to the theoretical limit do not allow compromises between key material properties. It is important to note that in solar cells functionality fully depends on intrinsic mechanisms related to transport of carriers from excited state s without an external driving force. It is important to distinguish between luminescent materials and devices and photovoltaic materials and devices. For luminescence trapping of excited carriers at localized potential wells could be helpful. For PV an undisturbed transport of minority carriers is essential. Microlectronic devices are mostly majoritycarrier devices, therefore these technologies can not serve as reference for photovoltaics . Whereas in majority carrier devices like field effect transistors mobilty is the key parameter, solar cells have to rely on minority carrier lifetime and diffusion length.

In devices graded bandgap could help to collect minority carriers and/or provide a barrier against recombination at contacts. Graded bandgaps are most beneficial with lattice matched alloy systems because of a low defect density.

For conversion efficiencies beyond the Shockley Queisser limit of a single junction it is essential to find a concept that allows exploiting all the energy of photon without sacrificing the performance of an optimized single junction solar cell. Modifications of ideal device structures could help to amend deficient material properties but will not help to go beyond theoretical limits of PV performance.

Since the number of single element semiconductors Si, Ge, Se and binary semiconductors (e.g. I_2-VI, II-VI, III-V compound is limited, the search for new materials goes along with an increased complexity of the compounds and device structures . This increased complexity on the one hand helps to tailor the material and devices, on the other hand could limit the performance due to inevitable inhomogeneities from deliberate introduction of functional nanostructures.

An obvious example for contradictory properties and misleading potential for improvement are amorphous semiconductors like a-Si:H. The disorder of the lattice on the one hand is a prerequisite for the increased optical absorption on the other hand the source for instabilities and band tails/defects as well as the limited mobility due to trapping processes at the mobility edge. It is important to be aware that improving a single property is not sufficient.

In devices with alternative concepts for solar energy conversion competing processes have to be carefully considered in particular with respect to the equilibrium and dynamics of charge carriers. Devices that rely on tunneling processes for the transport of photocurrents always suffer from losses of tunneling processes. Table 1 compares advantages and drawbacks of the different concepts of solar cells.

Table 1: Promises and drawbacks of different concepts for solar cells

concept	light absorption	photovoltage potential difference	transport carriers to selective contacts
homogenous semiconductor	indirect/ direct transition	appropriate band gap lifetime	mobility
quantum well 2d	high absorption localized transitions	imbedded in device structure band discontinuities	tunneling to get out of the well
3d quantum dots	high absorption localized transitions	imbedded in matrix band discontinuities	tunneling to get out of the well
intermediate gap	two levels , different energy, adjust absorption between levels	competing quasi fermi levels, recombination vs intermediate band	selective contacts for holes and electrons
hot electrons	higher energy photons	thermalisation	energy - selective contacts
plasmonic structures	absorption and transfer of photon energy		parasitic absorption
up/down conversion	confined spectrum		optical losses

In conclusion, present development of PV shows that best performance is obtained with optimized pn-junctions. Reaching module cost close to 0.25€/Watt the solar cell is getting a minor part of the cost of PV systems[iii]. So called low cost concepts always have to reach high efficiencies with a benchmark of 20%.

i Roadmap on optical energy conversion, S. V Boriskina et al, J. Opt. 18 (2016) 073004

ii P. Würfel, Physics of Solar Cells, Wiley 2009

Pathways for solar photovoltaics, V. Bulović et al., Energy Environ. Sci., 2015, 8, 1200.

iii Terawatt-scale photovoltaics: Trajectories and challenges, N. M. Haegel et al, Science 356 (6334), 141-143.