Photosteady State

One concept – many phenomena

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During my talk on the Quantsol winter workshop in Brigels last year we had a discussion about the energy level model which is a simplified depiction of the Jablonski diagram. We use this energy level model to explain phenomena like fluorescence and phosphorescence to pupils and students (see Fig. 1).

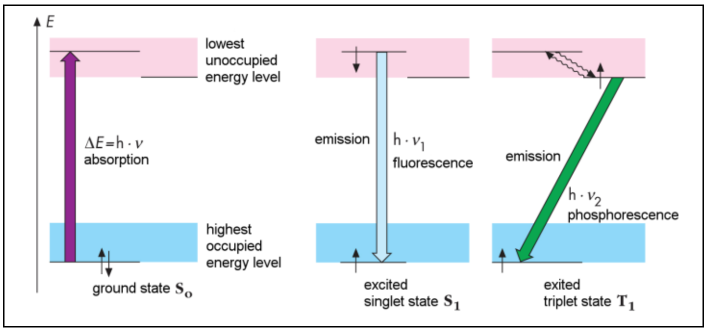

Fig. 1: Depiction of the energy level to fluorescence and phosphorescence

One disadvantage of this model is that only the energy levels of one molecule are shown. However, in a portion of matter there are many molecules, which can be in the electronically excited state or in the ground state.
Under irradiation the system reaches an equilibrium – the photosteady state, in which some molecules are in the ground state and some molecules are in the electronically excited state.

The distribution of the population between the electronically excited state and the ground state changes when irradiation is switched off.
The consideration of the population of states in the photosteady state and the processes which take place on the way from the photosteady state to the thermodynamical equilibrium lead to a deeper comprehension of many phenomena.
Phenomena like photochromism, fluorescence and phosphorescence, optical data storage, the seeing process and the generation of electric current in photovoltaic cells can be explained with one concept – the concept of the photosteady state.
The chemical substance spiropyrane will be picked out as a central theme of the talk.

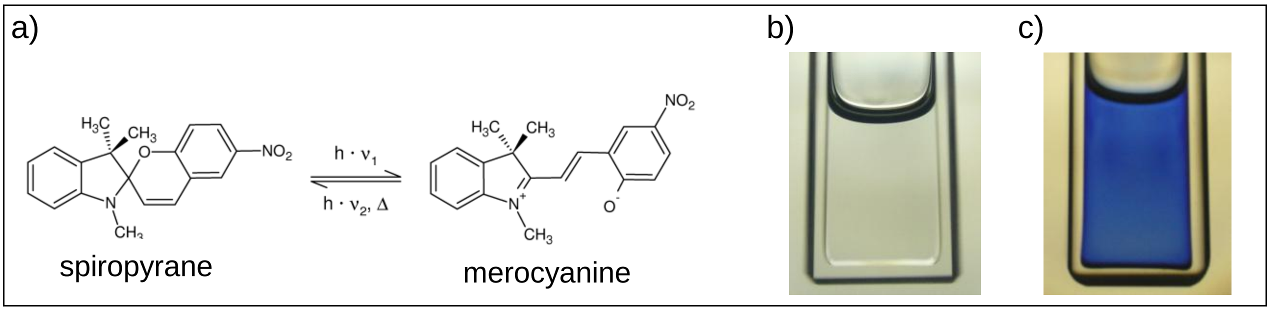

Fig. 2: a) Molecular structure of spiropyrane and merocyanine, b) spiropyrane in toluene before irradiation and c) spiropyrane/merocyanine after irradiation

We can teach the fundamentals of the concept of photosteady states with the photochromic system of spiropyrane in solvents or matrices where it acts as a molecular switch [1] (see Fig. 2). Pupils and students can investigate the dependence of the photosteady state and the transition to the thermodynamical equilibrium looking at different parameters (wavelength of the light, temperature and polarity of the solvent) in many experiments.

Besides significant experiments adequate depictions are required for the comprehension of the concept of photosteady states. A newly developed animation will be presented which helps to understand the photostationary state (see Fig. 3).

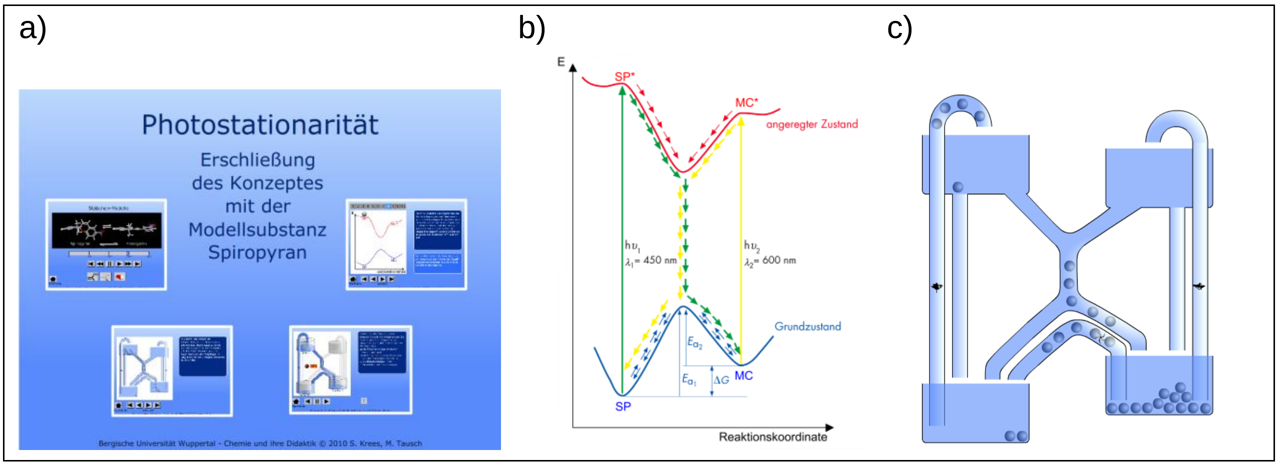

Fig. 3: a) Overview about the tools in the animation, b) energy potential hypersurfaces of the ground state and the electronically excited state for the reaction from spiropyrane to merocyanine, c) simulation model for the photosteady state

Different representations in the animation (structural models, pictographic models and two simulation models) include important aspects of the photosteady state. The animation goes beyond the simple model depicted in Fig. 1.

In a first tool of the animation the molecular structure of spiropyrane and merocyanine are shown in different model types which can be rotated to explore the difference in the molecular structures of the two isomers. The next tool shows the reaction pathway and the energy potential hypersurfaces of the ground state and the electronically excited state of the photochemical reaction from spiropyrane to merocyanine (see Fig. 3 b). Referring to the disadvantage of the model mentioned above two simulation models help to comprehend the concept of the photosteady state and the way from the photosteady state to the thermodynamical equilibrium.

In the first simulation the overlap and the synchronism of processes are shown with a certain number of molecules (see Fig. 3 c). The second simulation implements the transfer from the microscopic level to the macroscopic level. On this level we abstract from the molecular level and use the metaphor of flowing water as the portion of matter and water wheels and turbines as thermal and light energy.

[1] M. W. Tausch: „Ungleiche Gleichgewichte“, *Chemkon*, 3, **1996**, *3*, 123-127

[2] M. W. Tausch: „Excited states … the heart of all photoprocesses“, *Praxis der Naturwissenschaften - Chemie in der Schule*, 3, **2004**, *53*, 1

[3] Animation-Download under www.chemiedidaktik.uni-wuppertal.de
> Flash-Animationen > Photostationarität (English version is in preparation)