

Does singlet fission take place in tetracene dimer?

Bogomolov Alexandr S.,^{1*} Rogoveshko Vladislav M.,^{1,2} Baklanov Alexey V.¹

¹ Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Institutskaya 3, 630090, Novosibirsk, Russia

² Physics department, Novosibirsk State University, Pirogova 1, 630090, Novosibirsk, Russia

* E-mail: bogomolov.kinetics@gmail.com.

Singlet fission (SF) is a process of singlet exciton conversion into two triplet excitons which takes place in different materials. Big interest to SF is provided by the perspectives of its use in organic photovoltaics for conversion of solar energy into electric energy. The presence of SF provides enhancement of the quantum yield of triplet excitons which give rise to electron-hole pairs. According to the estimates by Hanna and Nozik [1] the use of this phenomenon can shift the so-called Shockley-Quisser limit for energy conversion efficiency to the higher values by 30%. This dictates the interest to the nature of SF phenomenon. The most studied SF materials are polyacenes. In theory the structural unit responsible for SF phenomenon is a dimer of polyacene. But the current studies of SF are mainly carried out not with the dimers but with the solid films which have complex structure which complicates the interpretation of experimental data. Another problem of the current studies that the SF process is detected indirectly as the decrease of luminescence yield and lifetime because it reflects the singlet exciton population.

In the presented work we study the formation of the triplet tetracene (Tc) excitons from the singlet exciton in Tc monomers and dimers isolated in molecular beam. Tc dimers and monomers are resonantly excited by pulsed dye laser in spectral range of $S_0 \rightarrow S_1$ transition. Further, the excited Tc molecules are ionized with a probing pulse of UV laser. Changing delay time between two laser pulses, we directly detect the short-living singlet excited states of Tc as well as long-living triplet states. We have found that triplet state of Tc with the same photoionization spectrum appears after excitation of both monomer and dimer of Tc. Taking into account that excitation of singlet state in monomer gives rise to triplet state via intersystem crossing (IC). We conclude that IC process can be a source of the observed triplet exciton in dimer as well. Moreover, this interpretation is also applicable to many experimental data from literature which were considered to be due to SF phenomenon.

The reported study was funded by RFBR, project number 20-52-12014.

[1]. M.C. Hanna, A.J. Nozik, *J. Appl. Phys.* **2006**, *100*, pp. 074510.