

# Kwansei Gakuin University

## Report of Research Outcome

2019/03/06

To President

Department : Science and Technology  
Position : Postdoctoral fellow  
Name : Li Wang

I report the outcome of the research as follows.

Name of the Fund/Program	<input type="checkbox"/> Sabbatical leave with grant <input type="checkbox"/> Sabbatical leave with no grant <input type="checkbox"/> KGU Joint Research <input type="checkbox"/> Individual Special Research <input checked="" type="checkbox"/> Postdoctoral fellow ※Please report by designated form as for "International Research Collaboration".
Research Theme	半導体ナノ微粒子系の多励起子素過程の解明と光応答分子システムへの応用
Research Site/Venue	Tamai Lab
Research period	2018/04/01 ~ 2019/03/31 ( 12 month)

◆ **Summary of the research outcome** (approx. 2,500 words)

Please write down the outcomes in detail regarding the research theme above.

**Research contents:**

Intramolecular singlet fission (iSF) is an efficient strategy of multiexciton generation for their applications of solar cells via one singlet exciton splitting into a correlated triplet pair in one organic molecule. Pentacene (Pc) dimers and polymers have been reported to be high quantum yields (QYs) of iSFs. However, there is no report on iSF of triangle acene derivatives in which one more available triplet site adjacent to the requisite two chromophores. In the case of tetracene (Tc) oligomers, only Tc oligomers with conjugated bridge represented high QYs of iSFs while not in the one with homo-conjugated bridge. We focused on the iSFs of Pc and Tc dimers and trimers with homo-conjugated bridge.

Steady-state absorption spectra of Pc and Tc monomers, dimers, and trimers represented similar spectra with several-nm red-shift in the oligomers, which indicated a negligible electronic coupling between the acene chromophores. Fluorescence QYs reduced from 46% and 87 % for Pc and Tc monomers to 7% and 49% for their dimers, and 3% and 32% for their

trimers. In both Pc and Tc derivatives, the fluorescence dynamics showed  $\sim 6.0$  ps decay components as compared with their long-lifetime monomers. Transient absorption (TA) spectra of Pc trimers represented fast relaxations at absorption peaks 463 and 1380 nm with rising signals at 516 and 973 nm, which were corresponding to the relaxation of singlet state and the formation of the triplet pair. The formation times of the triplet pair in the trimers (5.5 ps) were almost same to those in the dimers (6.0 ps), which suggested that an intermediated state should exist before the iSF process was triggered. Either a CT-state with an energy determined by the molecular morphology, or an exciton delocalization state barriered by the homo-conjugated bridge could be the intermediate state. The rate of this intermediate step was unique for the dimer and trimer owing to the same bridge. The available iSF site, that is the chromophore number, gives less influence on the reaction rates. Moreover, QYs of iSFs  $\sim 160\%$  in both Pc dimer and trimer could be directly obtained by analyzing TA of singlet state around 1380 nm in the near-IR region, which were in good agreement with the triplet sensitization experimental results. For Tc oligomers, solvent effects on iSF were monitored with increasing of polarity from 0.1 (hexane) to 4.6 (benzonitrile), and the rate of iSF in Tc trimers reduced from 0.18 to 0.33 ps<sup>-1</sup>, which suggested the charge-transfer state as the intermediate state in iSF of Tc dimer and trimer.

In summary, the intermediate state in iSFs of Pc and Tc oligomers with 2,3,2',3'-linkage were confirmed, and the homo-conjugated bridge influenced the formation time of the intermediate state and hence impacts on the reaction rate of iSFs. In Tc oligomers, the intermediate state was confirmed to be the charge-transfer state by its solvent effect on iSFs.

#### Conferences:

- 1) Li Wang, Sunna Jung, Toshiyuki Hamura, Naoto Tamai, "Intramolecular singlet fission in pentacene and tetracene oligomers, Annual meeting of photochemistry 2018, 3A07
- 2) Li Wang, Sunna Jung, Toshiyuki Hamura, Naoto Tamai, "Intramolecular singlet fission in acene dimers and trimers, Annual meeting of chemical society of Japan 2019, 3E02-39

#### Publications:

- 1) L. Wang, K. Nonaka, T. Okuhata, K. Tetsuro, and N. Tamai, "Quasi-Type II Carrier Distribution in CdSe/CdS Core/Shell Quantum Dots with Type I Band Alignment" J. Phys. Chem. C 2018, 122, 12038-12046
- 2) L. Wang, S. Takeda, T. Okuhata, R. Sato, T. Teranishi, and N. Tamai, "Ultrafast Spectroscopy and Coherent Acoustic Phonon of Au Nanopolyhedrons" (in draft)
- 3) L. Wang, S. Jung, T. Katayama, K. Kamada, T. Hamura, and N. Tamai, "Why the rate of intramolecular singlet fission in pentacene trimer is similar to the dimer?" (in draft)

Deadline : Within two months after finishing the research period.

Sabbatical leave with grant: Submit this report to President with confirmation by the dean of school you belong to.

※ Postdoctoral fellow is required to submit this report with confirmation by the dean of graduate school before the end of employment period.

Where to submit : Organization for Research and Development and Outreach (NUC)

◆ We put this report on the web of KGU. If there is any problem about it because of difficulties on your research, please let us know.