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様　式　C－7－1

令和元年度科学研究費助成事業（科学研究費補助金）実績報告書（研究実績報告書）

		機関番号	14603
所属研究機関名称		奈良先端科学技術大学院大学	
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1．研究種目名　特別研究員奨励費　　2．課題番号　19F19342

3．研究課題名　重励起子間相互作用による増強TADF分子の開発と円偏光発光OLEDへの展開

4．研究期間　令和元年度～令和３年度　　5．領域番号・区分　－

6．研究実績の概要

The goal of this project is to design new pure-organic TADF and CPL emitters for the development of new CP-OLEDs. Since CP-OLED is practically expected as a future candidate for highly efficient OLED with efficient light extraction efficiency. This is the cutting edge research target exploring efficient CP-OLED material and devices which are based on the thermally activated delayed fluorescence, TADF. This research is divided in two parts: synthetic organic chemistry and photo-physical analyses. At first, several molecular designs were discussed and various promising molecules, able to potentially form supramolecular structures, based on donor-acceptor patterns and including a substantial range of chiral moieties, have been selected. Multiple syntheses were conducted simultaneously. Following experimental observations and syntheses outcomes, some of the initial targets have been modified, redesigned and some synthetic pathways are presently being optimized. In the meantime, DFT calculations are performed for each targets and optimizations of the calculation methods are ongoing to get a realistic modelling of the singlet/triplet (delta-EST) energy gap and of the frontier (HOMO-LUMO) orbitals.

7．キーワード

TADF　CPL　OLED　fluorescence

8．現在までの進捗状況

区分　(2) おおむね順調に進展している。

理由

In the first part of this project, the synthesis of new targets was supposed to be the main focus of the research work. As expected, after thoughtful considerations of the design of the different targets, during those first 5 months I have focused on the syntheses of those emitters. The syntheses are still ongoing after optimization of the targets structures and after experimental observations. Soon photo-physical analyses should get started as well as optical spectroscopy and CPL measurements.

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９．今後の研究の推進方策

The synthesis of the design molecules will be pursued, completed and optimized. The photo-physical properties of the different targets will be investigated such as luminescence (absorption, emission, excitation spectra, time-resolved fluorescence spectroscopy, characterization of the TADF emission), IR and their CD/CPL nature. Each results will be thoroughly analyzed. Depending on the experimental results with comparison with the calculations performed, an optimization of the synthesized emitters: modification of the chiral moieties, modifying the donor and/or acceptor structure, introducing new chromophores to the structure, will be realized to obtain an increase in the desired performances. A discussion will be introduced with Prof. Reineke as Dresden, Germany aiming at promoting a future collaboration for the testing of the most promising emitters in OLEDs devices.

１０．研究発表（令和元年度の研究成果）

〔雑誌論文〕　計0件

〔学会発表〕　計0件

〔図書〕　計0件

１１．研究成果による産業財産権の出願・取得状況

計0件（うち出願0件／うち取得0件）

１２．科研費を使用して開催した国際研究集会

計0件

１３．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関			
フランス	ENS-Paris Saclay	－	－	－
－	－	－	－	－
－	－	－	－	－
－	－	－	－	－
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１４．備考

光情報分子科学研究室ーFaceBook
http://www.facebook.com/kawai.naist.jp