

PD Research Report for the 2016 year

Name (Research group) **Justyna Grabska (Ozaki lab, School of Science and Technology)**

Research Theme **Practical applications of quantum chemical calculations and numerical procedures to ultraviolet (UV) and far ultraviolet (FUV) spectroscopy of polymer nanocomposites**

Research Period **1.12 2016 - 31.03.2017**

Research Results (about 2,500 characters in Japanese, about 65 lines times 90 characters in English)

In December 2016 my first part of this research project was focuses on establishing the best approach for calculation of UV spectra of polymers. The main studied polymers: PDMS, PHB and PLA. And following candidates for possible extension of the above list: PET, PBT, PBS and PEL or PVPL. Owing for convenient structure, PDMS was chosen for establishing the best theoretical approach for calculation of electronic transitions and FUV spectra by TD-DFT method.

1. During this month the family of nylon polymers were studied as a reference molecular systems for further studies on other similar polymers (PHB, PLA, PET), since good literature data on nylons are available.
2. With the use of TD-DFT calculations (geometry optimization: B3LYP/cc-pVTZ; TD-DFT calculation of electronic transitions: CAM-B3LYP/ aug-cc-pVDZ) and using monomeric species as the object of studies, I have reproduced the data available in the literature with very good agreement.

I also attended in the conference Japan-Taiwan Medical Spectroscopy International Symposium, which was on Awaji Island and I have a poster presentation titled: 'Quantum mechanically calculated NIR spectra of fatty acids in applied studies'.