Usage Report for Fiscal Year 2019

Project Title: Development of Organic Semiconductors with Spontaneous Polarization

Name: ○**Daigo Miyajima (1), Cheng Zhang (1), Dan He (1)**

Laboratory at RIKEN:
(1) Center for Emergent Matter Science, Information Transforming Research Unit

1. Background and purpose of the project, relationship of the project with other projects

The design, synthesis, and characterization of new organic π-conjugated materials are crucial for the next-generation optoelectronic devices, such as organic photovoltaics, organic field-effect transistors, and organic light emitting diodes. These materials contain conjugated frameworks with high π-electron delocalization, being provided with unique optoelectronic properties. Nowadays, except for organic optoelectronic devices, ferroelectric devices with spontaneous polarization also require materials with conjugated frameworks with high π-electron delocalization in order to realize strong light absorption in NIR-vis-UV range to efficiently transfer solar energy to electricity, which is one of the hot topics recently. However, most of the organic materials are undeveloped and uninvestigated. In this case, we need to use theoretical methods like DFT calculation to estimate the conformation, HOMO/LUMO energy level, spin density, absorption spectra, intermolecular interactions, and so on. However, the π-conjugated materials usually have a large numbers of atoms such as C, H, O, N, which is very difficult to calculate by using simple personal computers. As a result, we need to use the supercomputer to support our calculation to guide our project.

2. Specific usage status of the system and calculation method

We usually need to use TD-DFT (time dependent density functional theory) method to calculate and evaluate our conjugated materials, and the software we use is Guassian 09 and psi 4.

3. Result

We designed and optimized several π-conjugated materials in our group, precisely evaluated the HOMO/LUMO energy level and absorption spectra of materials and thus successfully achieved the polar materials with strong light absorption in visible light region and could efficiently transfer solar energy into electricity. On the other hand, we successfully obtained a series of polar crystals from these designed π-conjugated materials. By using psi 4 calculation, we successfully calculate the intermolecular interactions between adjacent molecules and explained the mechanism of forming the polar crystals.

4. Conclusion

The theoretical calculation is very useful to support our project in the field of organic electronics and organic ferroelectric materials which we want to continue to use the supercomputer to support our further investigation.

5. Schedule and prospect for the future

2020/4-2021/3 Design new molecule systems and further evaluates the promising properties by theoretical calculation. Using theoretical calculation to further investigate the mechanism of unique properties of materials

6. If no job was executed, specify the reason.