Report for Interdisciplinary research startup

1. Name of project leader： **Yuriko Ono**
2. Project title: **Advanced Visualization of Reaction Route Network**
3. Report

Visualization of automated reaction pathway search results as graphs can provide an intuitive picture to help understanding of the entire chemical reaction routes. Following our previous work to reduce a dimension of a set of reference structures along the IRC by a classical multidimensional scaling (CMDS) approach (J. Chem. Theory Comput. 2018, 14, 4263), we proposed the method to project on-the-fly trajectories into a reduced-dimension subspace determined by the global reaction route map, using the out-of-sample extension of CMDS. As demonstration, the method was applied to the SN2 reaction, $OH^- + CH_3F$, and to the structural transformation of Au_5 cluster, which was accepted by JCTC.

Although the method of mapping the reaction path network for a few-atom system in two dimensions makes sense, it is difficult to employ this approach directly to a reaction type such as A + B → C + D or a dissociation into fragments, which appears commonly in catalysis and organic reactions. To extend the methodology to such a reaction type, we exchanged thoughts and ideas on the role of the reaction route maps in reaction design, with experimentalists and information scientists within ICReDD. There is a need to develop a notation that extracts important pathway information from complex reaction route maps and allows the experimentalists to search for similar reaction paths as for different compounds. Based on the knowledge and methods obtained in this project, we have just started a fusion study to speed up reaction development by using reaction pathway maps as knowledge sharing notes for reaction design.

To facilitate the creation of models that accurately represent the results of the calculations, a 3D printer was introduced in this project. I developed the program and set up environments to create the model properly. In combination with the reaction route maps, discussions using the model from the 3D printer could contribute to the development of new catalytic reactions.

4. Research achievement

- T. Taketsugu, T. Tsutsumi, S. Ebisawa, and Y. Ono, "Reaction path concept and dynamics effects: ab initio approach", International & Interdisciplinary Workshop on Chemical Reaction Dynamics - Mathematics Informatics, and Physics Meet Chemistry, Sapporo, 8 Oct, 2019.
- T. Tsutsumi, Y. Ono, Z. Arai, and T. Taketsugu, “Visualization of dynamics effect: projection of on-the-fly trajectories to the subspace spanned by static reaction path network”, J. Chem. Theory Comput., in press.