

Report for newly appointed faculty startup

1. Name of project leader : **Yuh Hijikata**

2. Project title: Theoretical investigation of potential of pore space in coordination polymer as reaction field.

3. Report

I conducted theoretical research aimed at fusion with information science in the future at ICReDD. The main use of the startup support was to construct my computing environment. Pore space of a porous coordination polymer in order to evaluate the potential as reaction fields, the interaction between molecules and a porous coordination polymer in or out of the pore is clarified by theoretical calculations[1]. I also attempted collaboration research with experimental researchers and published papers[2, 3], one of which led to international joint research. I am planning to use the results to incorporate information science in the near future.

4. Research achievement

[1] Coordinated water as new binding sites for the separation of light hydrocarbons in metal-organic framework with open metal sites; P. Veroots, A. Schnemann, I. Hante, J. Pirillo, Y. Hijikata, T. Toyao, K. Kon, K-i. Shimizu, T. Nakamura, S-i. Noro, R. A. Fischer; *ACS Appl. Mater. Interfaces*, 2020, 12, 9448 – 9456 (**Press Release**).

[2] Trans-influence across a metal–metal bond of a paddle-wheel unit on interaction with gases in a metal-organic framework; J. Pirillo and Y. Hijikata; *Inorg. Chem.*, 2020, 59, 1193 –1203 (**Supplementary Cover**)

[3] Topological molecular nanocarbons: All-benzene catenane and trefoil knot; Y. Segawa, M. Kuwayama, Y. Hijikata, M. Fushimi, T. Nishihara, J. Pirillo, J. Shirasaki, N. Kubota, K. Itami; *Science*, 2019, 365, 273 – 276 (**Press release**)