## Development of Efficient Triplet-DNP system Using Metal-Organic Frameworks

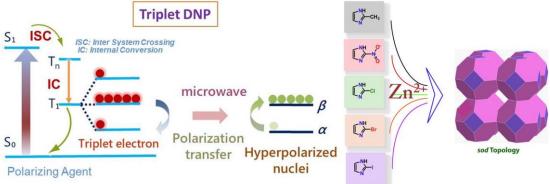
(<sup>1</sup>Graduate School of Engineering, Kyushu University, <sup>2</sup>Center for Molecular Systems (CMS), Kyushu University, <sup>3</sup>JST-PRESTO) O Arijit Mallick,<sup>1</sup> Saiya Fujiwara,<sup>1</sup> Hironori Kouno<sup>1</sup> Biplab Joarder,<sup>1</sup> Nobuo Kimizuka,<sup>1,2</sup> Nobuhiro Yanai<sup>1,2,3</sup>

**Keywords**: Dynamic Nuclear Polarization; Triplet Electrons; Nuclear Magnetic Resonance; Metal–Organic Frameworks; Host-Guest Chemistry.

NMR spectroscopy and MRI are powerful methods for the non-destructive analysis of microscopic structures and human body. Sensitivity of NMR and MRI is poor under the conventional conditions due to low nuclear spin polarization. In order to enhance the NMR/MRI sensitivity, dynamic nuclear polarization (DNP) has attracted great attention. High nuclear spin polarization has been achieved by using radical electrons as polarization source, but it requires the sample cooling to very low temperature around 1 K.

To overcome this problem, DNP using photo-excited triplet electrons becomes the focus of research. In triplet-DNP, hyperpolarization of nuclear spins can be achieve at room temperature by transferring triplet electron polarization to nuclear polarization. Presently triplet-DNP mainly uses dense host matrices. However, in order to not only polarize many kinds of molecules but also suppress the spin relaxation effectively, the development of new triplet-DNP system with accessibility of target molecules is required.

Here, we report a series of functionalized porous metal–organic frameworks with *sod*-topology<sup>[1]</sup> for triplet-DNP. We thoroughly studied the relationship between structure and spinlattice relaxation time of protons in these compounds, and then introduced polarizing agents into these frameworks. This would show <sup>1</sup>H NMR signal enhancement over thermal equilibrium.<sup>[2]</sup>



[1] R. Banerjee, A. Phan, B. Wang, C. Knobler, H. Furukawa, M. O'Keeffe, O. M. Yaghi, *Science*. 2008, 319, 939-943.

[2] S. Fujiwara, M. Hosoyamada, K. Tateishi, T. Uesaka, K. Ideta, N. Kimizuka, N. Yanai, *J. Am. Chem. Soc.* **2018**, *140*, 15606–15610.