“Properties of crystalline nano-cavities of metallo-macrocyle with dipeptide ligand”

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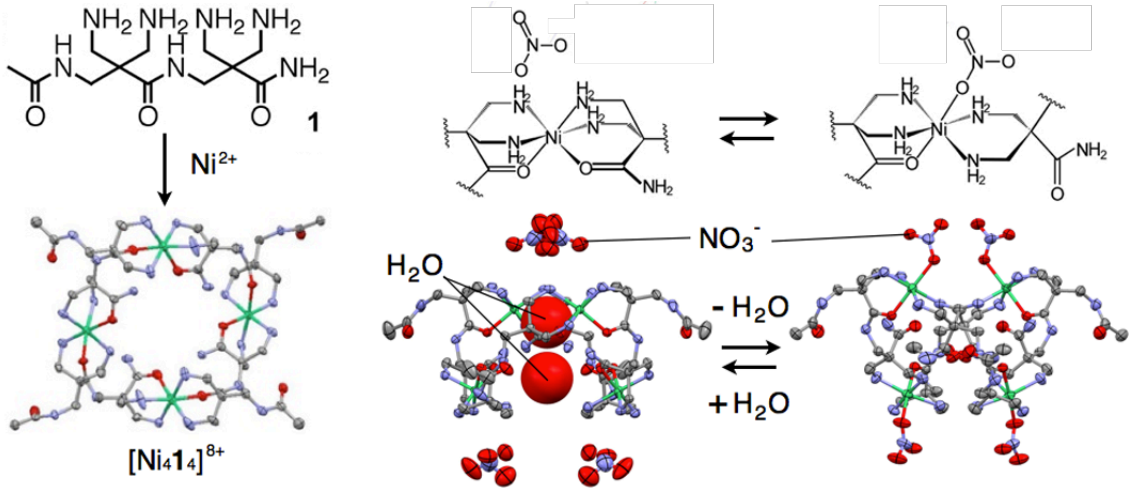
Towards designing sophisticated functions, we focus on developing metallo-macrocycles with peptide ligands because of their structural flexibility and high designable properties. We synthesized Ni(II)-macrocycles consisting of β-dipeptides with various counter anions (ClO_4^-, NO_3^-, BF_4^-, $CF_3SO_3^-$), possessing crystalline nano-cavities suitable for in-line arrangement of water molecules.

At first, we studied detail process of their water inclusion by single crystal X-ray analysis and thermal study to investigate dynamic properties of the macrocycles. We revealed that, in the case of NO_3 salt, release of included water molecules regulates the opening and closing of the cavities through cooperation of smooth ligand exchange and internal hydrogen-bond switching. This transformation undergo very smoothly above -40 °C by controlling surrounding temperature and humidity.

For their applications, we investigated their proton conductivities and gas adsorption properties. Although the diameter of nano-cavites is smaller than that of normal gas molecules, BF_4 salt adsorbed CO_2 gas with high selectivity.

In addition, to get designing strategies, counter anion effects on water arrangement and their reversible guest inclusion behaviors (including gas adsorption) in the crystalline nano-cavities were studied.



References

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