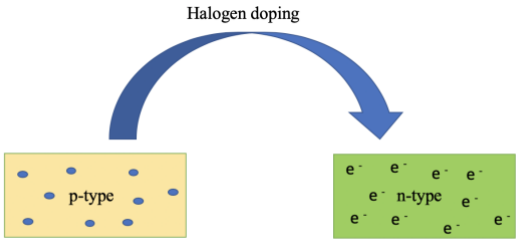
Effect of halogen doping on Electrical conductivity and Seebeck coefficient of metal-organic framework $Cu[Cu(pdt)_2]$ (pdt = 2,3-pyrazinedithiol)

([1]Graduate School of Science, Tohoku University) Shraddha Gupta,[1] Hiroaki Iguchi,[1] Shinya Takaishi,[1]

Keywords: Seebeck coefficient, pdt (2,3-pyrazinedithiol), Metal-organic framework

Metal-organic frameworks (MOFs) belong to a class of porous materials, formed by coordination bond between metal center and organic ligand. Amazing materialistic properties such as structural tunability, large surface area, long range order, chemical/thermal stability and tunable porosity allows MOFs for diverse applications in gas storage, separation and catalysis. However, a handful of report on electronic and electrical application of MOFs is due to its electronically insulating nature. Hence in order to promote conductive performance of MOFs some specialized strategies through which MOFs are modified is achieved. (e.g., via post synthetic modification or charge doping). In this work, a known three-dimensional MOF, $Cu[Cu(pdt)_2]$, with enhanced electrical conductivity was synthesized by doping halogens (iodine and bromine) into the pores. The increase in the electrical conductivity is due to the redox hoping between partially oxidized $Cu[Cu(pdt)_2]$ unit. In addition, the electronic and semiconductor properties of the MOF was studied by Seebeck coefficient measurement which reveals that in contrast to p-type characteristic of pristine MOF, the halogen doped MOF behaves as n-type semiconductor. This is caused by the band filling of the titled MOF. Powder X-ray diffraction (PXRD) analysis was performed in order to check the effect of encapsulation of halogens on the crystallinity of host MOF, the framework structure did not change with, whereas peak intensity changed with increasing concentration of halogen inside the MOF. To this end we have presented the framework which shows the switchable behavior from p-type semiconductor to an n-type semiconductor as result of halogen doping.



Schematical representation of conversion of p-type pristine MOF to n-type doped one.

References:

1. S. Takaishi *et al.*, *Inorg. Chem.* **2009**, 48, 9048–9050
2. Y. Kobayashi *et al., Chem. Mater.* **2010**, 22, 4120–4122
3. S. K. Bhardwaj *et al., J. Mater. Chem. A,* **2018**, 6, 14992–15009