

## Metallo-Supramolecular Polymer Synthesis Driven by Data-Science

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Materials informatics has received much attention recently as a powerful tool to develop materials. In general polymer materials are composed of monomers and the selection of the monomers decides the chemical and physical properties of the polymers. In addition, the degree of polymerization is also an important factor to influence the properties of the polymers. If materials informatics is successfully introduced to the polymer design, polymers with desired properties will be synthesized efficiently. In this presentation we report our recent approach on the search of electrochromic (EC) metallo-supramolecular polymers (MSPs) with the help of materials informatics.

MSPs are synthesized by complexation of metal ions and multitopic organic ligands. The obtained polymer chains are composed of successive metal complex moieties, which often have a metal-to-ligand charge-transfer (MLCT) absorption. We revealed the reversible switching of the disappearance/appearance of the MLCT absorption triggered by the electrochemical redox of the metal ions.<sup>1</sup> The EC properties were evaluated from viewpoints of the wavelength of the MLCT absorption and the redox potential, the contrast, the switching speed, and the coloration efficiency (CE) etc. To improve the EC properties, the polymer components should be suitably selected. However, the present research to find better EC polymers is based on our experience and serendipity, because the number of the components is too many to synthesize all the polymers with the combination of the components. To overcome the issue, materials informatics was introduced.

Four components were selected among many components of MSPs such as the metal species, the counter anions, and the ligand structures, and several variations on the chemical structures were chosen regarding each component. Among all the combination of the variations, the selected number of the corresponding MSPs according to an orthogonal table were synthesized. The obtained polymers showed significantly different EC properties and it was found that this method with statistics was useful to find the polymers with better EC properties quickly. The detailed information on the selected components, the structural variations, and the combinations in the polymer synthesis, and the measurement results on the EC properties will be explained in this presentation.

### References.

- 1) M. Higuchi, *J. Mater. Chem. C*, **2014**, 2, 9331 (Feature article).