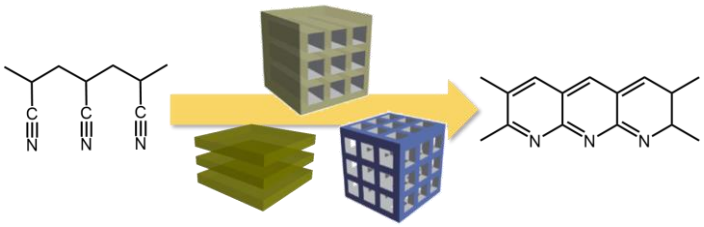
Carbonization of Polyacrylonitrile Chains in Metal-organic Frameworks

([1]*Graduate School of Frontier Science, The University of Tokyo*, [2]*Graduate School of Engineering, Kyoto University,* [3]*Graduate School of Engineering, The University of Tokyo*)
○Xiyuan Zhang,[1] Ryoto Hongu,[2] Takashi Kitao,[1,3] Takashi Uemura,[1,3]
Keywords: Polyacrylonitrile; Metal-organic Framework; Radical Polymerization; Carbon Materials

Carbon materials have been extensively used in various applications, including catalysts, energy storage, and carbon fibers, because of their outstanding physical properties. Polyacrylonitrile (PAN) is one of the most widely applied precursors to fabricate carbon materials. Although great effort has been paid for decades to control carbonization reaction of PAN, the detailed reaction mechanism still remained unclear due to its random and complex entanglement of the polymer chains in the bulk state.[1] Furthermore, the carbonization reaction is an exothermic process with the rapid evolution of heat, which provokes unfavorable side reactions and scission of the polymer chains; thus the process of carbonization reaction is difficult to control in the bulk state.

Confinement of polymer chains in porous materials is a feasible method to prevent the entanglement and conformational disorder occurring in bulk polymers, allowing regulation of their assembly structures. Carbonization reaction of PAN chains within well-defined nanospaces should provide insight into effect of aggregation structures of PAN on their carbonization reactions. For this purpose, we employed metal−organic frameworks (MOFs) prepared by the self-assembly of metal ions and bridging organic ligands, which offer a wide range of applications, such as gas separation, storage, and catalysts. The regulated and tunable nanopores of MOFs can allow us to achieve precise control of polymer assemblies accommodated in the nanochannels.[2] Here, we encapsulated PAN in MOFs by in-situ polymerization, and subsequently thermal transformation to investigate the confinement effect on the resulting structure of carbon materials.[3]



REFERENCES

1) M. S. A. Rahaman, A. F. Ismail, A. Mustafa, *Polym. Degrad. Stabil.*, **2007**, *92*, 1421.
2) T. Kitao, Y. Zhang, S. Kitagawa, B. Wang, T. Uemura, *Chem. Soc. Rev*. **2017**, *46*, 3108.
3) X. Zhang. T. Kitao, D. Piga, R. Hongu, S. Bracco, A. Comotti, P. Sozzani. T. Uemura, *Chem. Sci*., **2020**, *11*, 10844.

© The Chemical Society of Japan