Data-driven polymer design toward circular economy system

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The recent development of sequence-engineering in synthetic copolymers has led to the innovation of polymer materials. Short sequences, referred to as "codons" using an analogy to nucleotide triads, play crucial roles in expressing functions. However, the lack of efficient sequencing methods prevents the experimental determination of codon compositions, which hinders the integration of experiments and theories. To overcome this, a polymer sequencer based on mass spectrometry of pyrolyzed oligomeric fragments is proposed. Despite random fragmentation along copolymer main-chains, the characteristic fragment patterns of codons are identified and quantified through unsupervised learning of a spectral dataset of random copolymers. Codon complexities increase with length and monomer component number. By expanding the dataset, the data-driven approach accommodates the increasing complexities, enabling the quantification of codon compositions of binary triads, binary pentads, and ternary triads with small datasets (N<100). The sequencer can describe copolymers with their codon compositions/distributions, facilitating the sequence-engineering of innovative polymer materials. In this presentation, we will introduce our recent efforts to develop data-driven polymer materials using materials informatics and polymer smart labs.

References

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