Machine Learning-Assisted Design of Full-Color Fluorescent Polymers

Yinyin Bao

Institute of Pharmaceutical Sciences, Department of Chemistry and Applied Biosciences, ETH Zurich, Vladimir-Prelog-Weg 3, 8093 Zurich, Switzerland
Email: yinyin.bao@pharma.ethz.ch

Tuning the emission color of fluorescent materials in solid state is of great interest for both fundamental research and practical applications.[1] However, it is rather challenging to develop full-color polymers that have simple structure and are easy to synthesize. We recently discovered the possibility of manipulating excited states of single fluorophore-polymer conjugates via polymerization-mediated through-space charge transfer (TSCT).[2] Consequently, variation in solid-state emission color was observed. Here, directed by a machine learning model based on previously synthesized polymers, we report a versatile polymer platform with full-color emission tunability.[3] Using a single-fluorophore acceptor as the initiator, a series of electron-donor groups containing simple polycyclic aromatic moieties were introduced by facile copolymerization or post-functionalization. In line with the prediction results, the *de novo* designed TSCT polymers showed continuously tunable emission color (Figure 1). Theoretical investigations confirmed the structurally dependent charge transfer-induced emission redshifts. We further demonstrated this polymer platform can be used to design solid-state stimuli-responsive materials for light-controlled information encryption.

Figure 1. Photographs of TSCT polymers from various polycyclic aromatic monomers

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