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1.Evaluation of O_2 Diffusion within Amorphous Polymer Films under Low Temperature via Phosphorescent Imide Compound

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Abstract: Gas permeability in amorphous polymer films at low temperatures is crucial for the development of gas separation/barrier membranes and packaging materials for low-temperature storage. The objective of this research is to clarify the mechanism of O_2 diffusion under low temperature by observing variable-temperature photoluminescent (VT-PL) measurement with phosphorescent imide compound (PH-Im, **Figure 1**).

VT-PL spectra of PH-Im-dispersed polystyrene (PS) and polyethersulfone (PSF) films were measured under an O_2 atmosphere from 300 to 100 K. The PH intensity increased with decreasing temperature, reflecting the suppression of O_2 diffusion[1]. The activation energy (*Ea*) for PH enhancement was estimated to be 27.8 kJ/mol for PSF, whereas PS showed two Ea values: 20.8 kJ/mol (300–200 K) and 11.5 kJ/mol (200–100 K). O_2 permeability (P_{O2}) was also measured by the constant-volume/variable-pressure method from 200 to 360 K. The E_a for P_{O2} was 25.0 kJ/mol for PSF, whereas PS exhibited two distinct E_a of 22.9 and 6.31 kJ/mol.

The close agreement between VT-PL and P_{O2} measurements confirms that VT-PL can serve as a new *in-situ* technique for evaluating O_2 diffusion in amorphous polymers at low temperatures. Additionally, molecular dynamics (MD) simulations further suggested that O_2 diffusion occurs via hopping between free-volume sites, which is assisted by local polymer-chain motion[2]. Thus, O_2 diffusion at low temperatures is correlated with the polymer-matrix mobility.

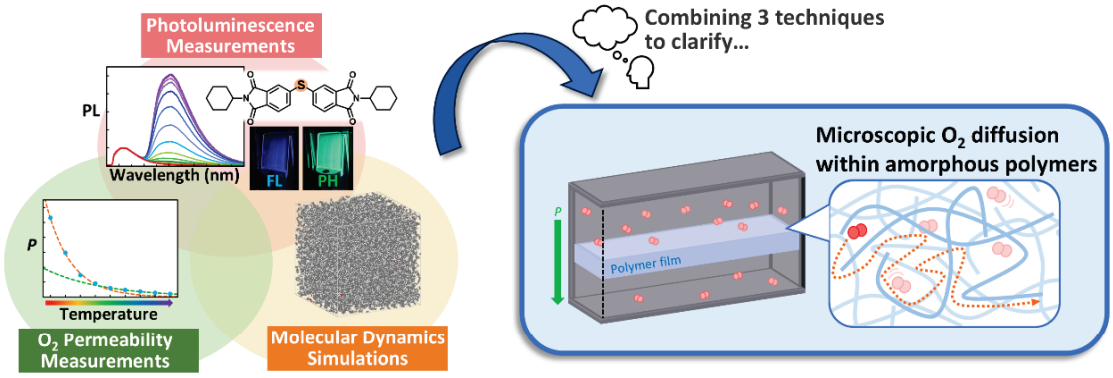

Figure 1 Schematic graph of research objective and experimental methods.

Key words: phosphorescence, O_2 diffusion, low temperature, amorphous polymers

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