学 位 論 文 の 要 約

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学 位 論 文 題 名

Design of Underwater Adhesive Hydrogels through Bioinspired Data-Driven Strategy
（バイオインスパイアードなデータ駆動型戦略による水中接着性ハイドロゲルの設計）

This dissertation presented a data-driven approach to the design of high-performance underwater adhesive hydrogels, leveraging insights from natural adhesive proteins and machine learning techniques. The main findings of this research are summarized as follows:

1. Bioinspired Design through Data Mining: We developed a comprehensive data mining strategy to extract adhesion-related sequence patterns from natural adhesive proteins. These patterns guided the formulation of 180 protein-inspired hydrogels, forming the foundation for a scalable training dataset.

2. Optimized Adhesion Performance via Machine Learning: Based on the data mining results, ideal random copolymerization was employed to statistically replicate their characteristic sequence heterogeneity, thereby constructing a training dataset. Machine learning techniques were subsequently applied to optimize hydrogel formulations, leading to the discovery of super-adhesive hydrogels with adhesion strengths exceeding 1 MPa. These optimized hydrogels demonstrated superior performance across diverse substrates and aqueous environments.

3. Ionic-Aromatic Motifs for Enhanced Electrostatic Interactions: Inspired by the salt bridge motifs in natural proteins, we introduced ionic-aromatic motifs into synthetic polymers, significantly stabilizing electrostatic interactions even in high-salinity environments. This strategy not only enhanced the underwater adhesion but also enabled efficient adsorption of ionic contaminants.

In conclusion, this dissertation provides a systematic, scalable, and data-driven framework for the design of high-performance underwater adhesive hydrogels. The integration of data mining, machine learning, and bioinspired design principles offers a promising approach for developing next-generation functional materials. Future studies will aim to further enhance adhesive performance on diverse substrates and extend the application of this strategy to other functional soft materials.