学 位 論 文 内 容 の 要 旨

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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）

Underwater adhesives with instant, robust, and repeatable adhesion have transformative potential across various fields, yet their development remains a significant challenge due to the disruptive effects of water at the interface. The vast biological knowledge embedded in organisms capable of adhering to wet or underwater surfaces provides a rich source of inspiration for the design of underwater adhesives. The recent progress of data-driven methodologies has provided powerful tools for large-scale information analysis, significantly aiding materials development. However, their application to soft materials remains challenging due to the inherently complex and multiscale structure–property relationships. Drawing inspiration from natural soft materials, we propose a data-driven framework that integrates data mining, experimental, and machine learning to accelerate the development of high-performance soft materials. Here, this proof-of-concept study showcase the success of our data-driven framework in de novo developing super-adhesive hydrogels from scratch, tailored for demanding underwater environments. Knowledge discovery from adhesive protein databases, we devised a descriptor strategy to statistically replicate protein sequence patterns in polymer strands through ideal random copolymerization, enabling targeted hydrogel design and dataset construction. Using machine learning, we optimized hydrogel formulations from an initial dataset of 180 bioinspired hydrogels, achieving a remarkable improvement in adhesive strength, with a maximum value exceeding 1 MPa. Moreover, we introduced a salt bridge-inspired ionic-aromatic motif strategy to stabilize electrostatic interactions, further improving adhesion and enabling efficient adsorption of ionic contaminants in high-salinity environments. This work offers a scalable, systematic, end-to-end approach for developing a wide range of functional soft materials, opening new possibilities in various fields.