Introduction of Data Science in the Development of Electrochromic Polymers

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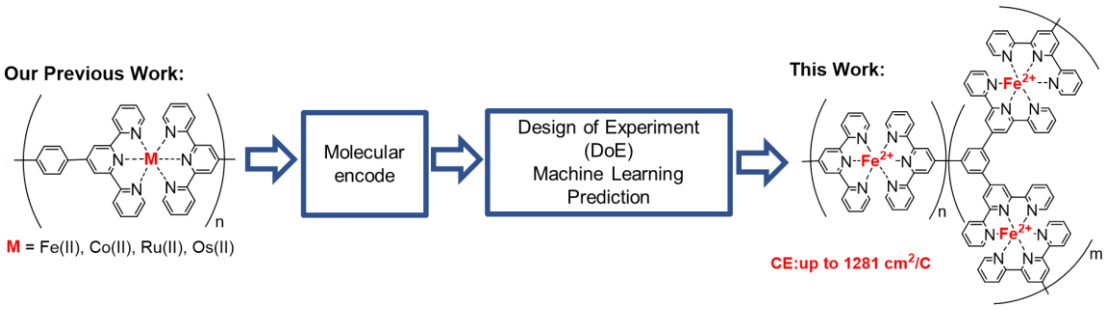
Materials informatics has emerged as a powerful tool for developing functional materials, offering the potential to streamline polymer synthesis with tailored properties, enhancing efficiency and specificity in material engineering. Machine learning, a subset of AI, uses algorithms to learn from data for predictions or decisions.[1] Bayesian optimization, widely used in materials science, optimizes objective functions and is particularly useful in hyperparameter tuning for machine learning models.[2]

In this presentation, we report our approach to discovering electrochromic (EC) metallo-supramolecular polymers (MSPs) using materials informatics. Four MSP components were evaluated, and selected combinations synthesized via an orthogonal table. Four machine learning model categories, including tree-based, kernel-based, linear, and neural network models, were trained to predict MSP properties effectively. This study achieved a high coloration efficiency of 1281 cm^2/C, which surpassed the values reported in our previous study.[3] This statistics-based approach demonstrates its effectiveness in the rapid identification of polymers with enhanced EC properties.



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