ORGANIC SEMINAR

Autonomous Discovery of Electrochromic Polymers

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The design of functional polymers, from desired functionalities to specific structures, has long faced challenges in balancing accuracy and efficiency. Dealing with this dilemma, a more effective method for knowledge accumulation, polymer property prediction, and experimental validation is required. To tackle these challenges, we developed Polybot, an artificial intelligence-empowered robotic laboratory that facilitates such inverse design. Employing advanced tools like large language models and figure digitalizing programs, Polybot rapidly constructs a database by extracting polymer structures, properties, and synthesis conditions from textual and graphical literature sources. By introducing copolymer Set-Transformer, a physics-informed machine learning model created for copolymers, into the autonomous laboratory, Polybot realized autonomous on-demand polymer synthesis, achieving desired electrochromic functionality with unparallel accuracy and efficiency.

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