Accelerating materials innovation through automated theoretical-experimental iterations empowered by AI-Chemist

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Abstract Body:

Advances in high-performance computing, artificial intelligence, and robotics are transforming the traditional trial-and-error paradigm of chemical research to a new era. The gap between theory and experiment remains a key barrier: theoretical datasets are large but over-idealized, while experimental data capture real-world complexity, yet are limited in size. We present an automated theoretical–experimental iteration framework empowered by AI-Chemist. Universal ML interatomic potentials act as a surrogate calculator, efficiently generating large-scale theoretical data leveraged by automated computational workflows. Reinforcement learning is employed to optimize experimental sampling strategies, while theoretical and experimental data are integrated into a unified ML model for calibration and refinement. The closed-loop approach systematically resolves discrepancies between theory and experiment, yielding increasingly reliable predictive models. By tightly coupling automated computational workflows, automated machine learning, and robotic experimentation, the framework accelerates the design–test–learn cycle and establishes a self-evolving ecosystem and we envision such systems as the foundation of next-generation autonomous laboratories for chemistry and materials innovation.