Accelerating Materials Discovery Using Machine Learning Techniques for Renewable Energy and Sustainability Solutions

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Advanced materials are key to the ongoing transition towards renewable energy and sustainability. Computational chemistry techniques enable the accelerated discovery of materials by speeding up exploration, providing mechanistic insights, and reducing costs compared to experimental research alone. Particularly promising approaches for accelerating computational discovery include machine learning (ML) and reasoning-based artificial intelligence (AI).[1,2]

Recent examples of materials discovery enabled by ML and AI in the areas of catalytic CO_2 reduction and the screening of materials for CO_2 capture and biohydrogen purification will be presented. For catalyst discovery, we employ supervised ML models and propose ML-enhanced descriptors based on the Fukui function. To illustrate the reliability of the approach, we analyze the correlation between the proposed descriptors and the surface binding energy of CO. Our results show that the Fukui function, augmented by the surface work function, is well correlated to the mapped binding energy of CO and might replace the computationally expensive energy mapping using density functional theory (DFT), as an indicator of catalytic activity.[3] For CO_2 capture using amine-based solvents, we have conducted a benchmark study of semiempirical methods to identify an approach that reproduces the trends predicted by the DFT calculations. The results show that, despite the limited direct correlation between the semiempirical PM7 and DFT values, trained regressors incorporating both geometrical and electronic features capture the underlying nonlinear patterns and significantly improve predictive accuracy. The demonstrated workflow provides a viable pathway to reduce the computational cost of modeling CO_2 capture systems.[4] For H_2 purification, we have demonstrated a comprehensive high-throughput screening of metal-organic frameworks (MOFs) from the CoRE MOF database to identify optimal candidates for CO_2/H_2 separation from biogas under common pressure and vacuum swing adsorption conditions. Molecular simulations and DFT are employed to evaluate separation descriptors across pressure regimes. The performance ranking of MOFs is determined according to an overall score, which integrates metrics, such as MOF working capacity and CO_2-adsorption selectivity, toward a binary gas mixture. This robust computational framework is intended to guide the rational design of next-generation adsorbents for renewable biohydrogen production.[5]

The Theory of Inventive Problem Solving (TRIZ) has been employed for systematic innovation in engineering and materials science. We have proposed a novel framework that integrates the logic-based principles of the TRIZ with large language models (LLMs) to emulate researcher-like reasoning in atomistic materials science. This approach not only amplifies current trends in physics-informed ML and generative design but also democratizes advanced problem solving to accelerate discovery toward ideality.[2]

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