AI-Enhanced Computational Chemistry for Energy Applications: Sensors, Batteries, and Catalysts

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ABSTRACT

Recent advances in AI-driven materials simulation are transforming our ability to efficiently explore the virtually infinite materials space. Machine-learning potentials (MLPs), which retain near–density functional theory (DFT) accuracy while accelerating computation by several orders of magnitude, have emerged as a particularly powerful approach. Trained to predict energies directly from atomic configurations, MLPs are rapidly evolving from system-specific models to universal frameworks capable of learning bulk, surface, amorphous, and adsorption structures within a single integrated model. These universal MLPs now achieve more than 97 percent accuracy in energy stability prediction and enable large-scale simulations that were previously inaccessible due to the limitations of conventional computational resources. In this seminar, I will first outline key challenges in energy-related fields, including chemiresistive gas sensors, all-solid-state batteries, and electrocatalysis, through representative examples of DFT and classical molecular dynamics approaches. I will then introduce how recent developments such as universal MLP methodologies can address these challenges by dramatically accelerating simulations and expanding the materials space.