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Contribution ID: **3204** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Pushing the length and time scales of AIMD

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Molecular Dynamics (MD) is a commonly used technique to simulate the evolution of atomic structures and complex materials. MD based on classical force fields can solve large systems with relatively long time scales. Since the accuracy of MD depends on the quality of the underlying force fields, and there are many situations where complex chemical reactions occur due to electronic interactions, an important research direction is to advance the method of Ab Initio Molecular Dynamics (AIMD) based on the self-consistent Kohn-Sham density functional theory (KS-DFT), to larger length and time scales.

In this work, we present an accelerated AIMD which harnesses its power by two approaches. First, the AIMD is based on our real space KS-DFT method RESCU [1] which can efficiently solve supercells containing many thousands of atoms. Second, we leverage Gaussian Process Regression (GPR) to efficiently extrapolate forces by interpolating between KS-DFT calculations from previous timesteps in the AIMD simulation. By extrapolating forces via GPR when possible, and only calculating forces via KS-DFT when necessary, novel reactive dynamics on increasingly large timescales can be studied using modest computational resources. The accelerated AIMD is applied to simulate the Solid Electrolyte Interphase (SEI) formation in a 2590-atom system consisting of an interface between a lithium slab and liquid organic electrolyte, to time scales of a picosecond or more, where important chemical reactions at the solid/liquid interface are identified.

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