Type: New
Title: "Million Atom Chemical Dynamics at Heterogeneous Aqueous Interfaces"

Principal Investigator: Roberto Car, Princeton University
Co-Investigators: Lin Lin, University of California, Berkeley
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Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (720,000 Summit node-hours)

Research Summary: Molecular processes in aqueous solutions in contact with solid interfaces are central to geochemistry, biology, and energy technologies. Car's team is working to better understand these phenomena, which would make a significant step towards better controlling them, an issue of substantial societal impact. Computational modeling, specifically the use of Summit, is essential to accomplish this task because complexity and disorder makes it difficult to extract precise microscopic information from experiments.

Car's team will use Summit to model millions of molecules at the level of quantum mechanics for tens of nanoseconds. They will perform ground-breaking molecular dynamics simulations to study mass/charge transfer processes at a prototypical interface of titania (TiO_2) with aqueous solutions of varying pH and excess salt concentrations. The deep potential molecular dynamics (DPMD) method, developed at Chemistry in Solution and at Interfaces (CSI), makes use of modern artificial intelligence techniques to learn from accurate but costly quantum mechanical calculations the complex way in which the energy and charges of a multi-atom system depend on the system coordinates. By harnessing the computational power of Summit, DPMD makes possible million-atom simulations for time spans of up to hundreds of nanoseconds, while retaining quantum mechanical accuracy essential for modeling chemical dynamics. The proposed simulations will use 1 million water molecules and 100 thousand TiO2 units with varying acid (HCl), base (NaOH), and excess salt (NaCl) concentrations, to study how the pH gradients affect the ionic charge distributions in the solution and at the solid interface.