MOSAIC: Materials Optimization and Simulation by Ab Initio Computation

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The MOSAIC group develops and applies molecular and submolecular computational models to understand, predict, and maximize the performance of materials for energy conversion and storage. By implementing computational techniques such as large-scale finite temperature models, multiscale electrochemical models, beyond-DFT electronic structure methods, data-intensive screening workflows, and interpretable machine learning, we investigate novel materials such as efficient semiconductor photo-electrodes for hydrogen production, high selectivity electrocatalysts, efficient light-absorbing layers and transparent conducting films for solar energy technologies, and next-generation ferroelectrics for post-von-Neumann microelectronics working at the interface between materials science, physics, and chemistry in collaboration with experimentalists.