



Award #: 1835690

CSSI Elements: Software: **Autonomous, Robust, and Optimal In-Silico Experimental Design Platform for Accelerating Innovations in Materials Discovery**

PI: Byung-Jun Yoon¹, Co-PIs: Raymundo Arroyave², Xiaofeng Qian², Xiaoning Qian¹

¹Dept. of Electrical & Computer Engineering, ²Dept. of Materials Science & Engineering, Texas A&M University

- This project aims to design & implement a **robust and optimal *in-silico* experimental design platform** and to provide a preliminary demonstration of its applicability for **autonomous simulation-based materials discovery**
- Focus is on an innovative **Bayesian learning/experimental design framework based on MOCU** (mean objective cost of uncertainty) that enables (1) integration of data, scientific knowledge, and first principles in materials science, (2) goal-based uncertainty quantification and optimal experimental design

Research Progress Highlights

- Machine learning scheme for **automated feature engineering** that can find (1) *physically meaningful features* (2) that can *accurately predict functional properties*
- Active learning** scheme for *efficient sampling of configuration space* for developing density-functional theory (DFT)-based machine learning force field (MLFF) for large scale molecular dynamics (MD) simulations

