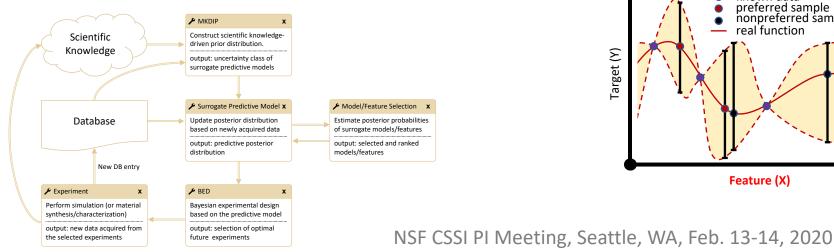


CSSI Elements: Software: Autonomous, Robust, and Optimal In-Silico Experimental Design **Platform for Accelerating Innovations in Materials Discovery**

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- 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** ٠ 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

