

## Sequential Experimental Design

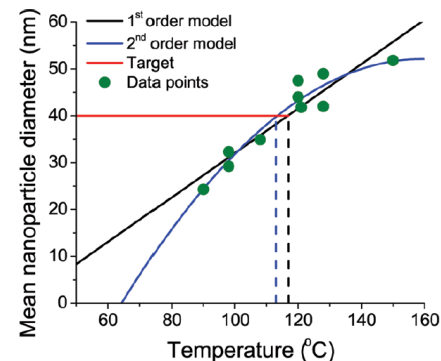
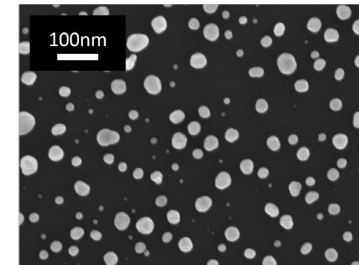
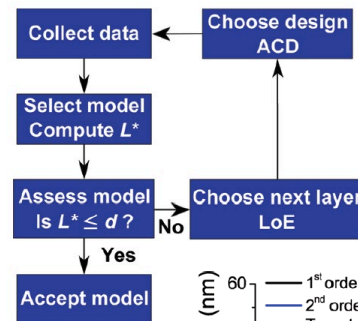
*J. C. Lu*, Stewart School of Industrial and Systems Engineering  
*Martha Grover*, School of Chemical & Biomolecular Engineering  
*Dennis Hess*, School of Chemical & Biomolecular Engineering

**Objective:** Execute the most informative experiments by synthesizing all available knowledge and by formally specifying the goal of the experiment. Physics-based models are utilized when available, together with expert opinion, literature data, and experimental data.

**Technical Approach:** Statistics provides the comprehensive framework from which to integrate all sources of knowledge. Learning is enabled via feedback~.

- The objective of the experiment is formally defined, which may be to build a model, or as shown in the figure, to identify a recipe to meet a target property.
- A comprehensive model is built utilizing information from literature data, experimental data generated by the project, and expert opinion (potentially solicited through surveys). This information is combined with a hypothesis set which may include physics-based models. Machine-learning is used to build a comprehensive model and simulator of the process. A set of experiments is designed, to maximize the objective. Methods include adaptive combined design (ACD) and layers of experiments (LoE).
- New experimental data is collected and used to update the model, design and conduct new experiments, etc. until the target property is achieved with desired statistical confidence level.

### Concept Illustration:



**Impact:** Optimal recipes can be identified, with statistical confidence, improving material performance while simultaneously reducing the number of experiments needed to optimize the recipe. Physics-based models can be exploited if available, but the experiments proceed in either case, utilizing all available information in a systematic framework.

