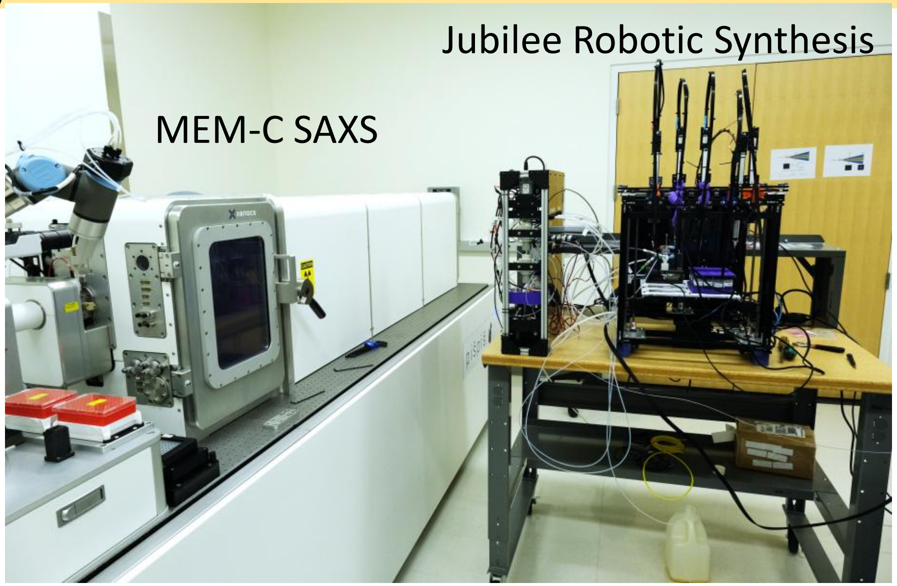
UW MRSEC
DMR-2308979

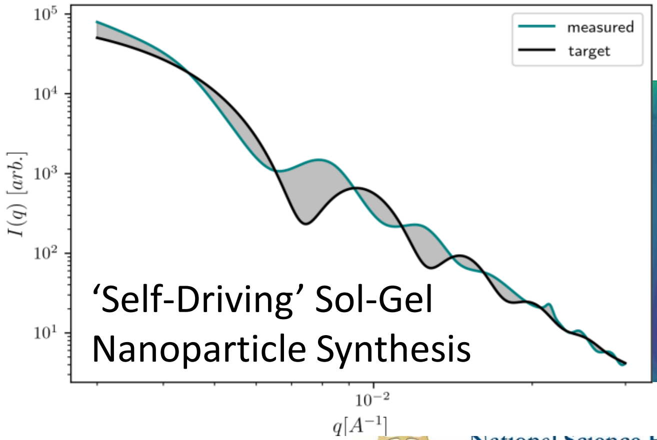
MEM-C's Artificial Intelligence (AI) Core Activities

Pozzo (Seed, IRG-1), Jameison (Seed), Sun (Seed), Dunham (IRG-1), Cao (IRG-2), D. Xiao (IRG-2)

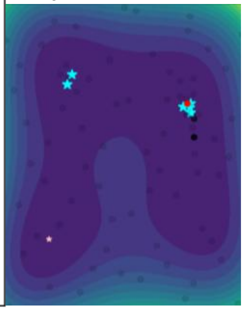
MEM-C's AI Core is working across Seeds and IRGs leveraging emerging machine-learning (ML) methods to speed materials development. Activities include:

- **Developing and integrating 'self-driving laboratory' capabilities into MEM-C user facilities (Pozzo, Jameison, Sun)**
  - Using robotic systems with MEM-C's small-angle X-ray scattering (SAXS) user instrument to optimize nanoparticle syntheses.
  - Approach developed and tested using nanoporous SiO_2 colloids (pictured) and ZnO nanoparticles with a flow-through synthesis approach (not shown) that integrates band-gap measurements.
  - These capabilities will accelerate the process of developing new syntheses that deliver target nanoparticle structures and properties.
- **Building deep learning models based on DFT calculations for predicting defect properties in cubic semiconductors (Dunham) [1]**
  - Models identify new dopant species to optimize device performance.
  - Validated *via* existing experimental observations and DFT.
  - Predictions implemented in TCAD to quantify and optimize device impact.
- **MEM-C's AI Core (Jameison, Cao) led roundtables to identify opportunities.**
  - Education of faculty, students and post-docs on ML capabilities.
  - Brainstorming and lightning talks to identify target applications.
- **Using ML force fields trained on DFT calculations (Cao, Xiao) to perform large-scale structural relaxations of twisted bilayer TMDs across twist angles. [2,3]**





Bayesian Optimization



[1] X. Xiang, D. Soh, and S. Dunham, *JPCC* ***128*** **(21)**, 8821 (2024).
[2] X.W. Zhang, C. Wang, X. Liu, et al. *Nat Commun.* **15**, 4223 (2024).
[3] E. Thompson, K.T. Chu, et al. https://arxiv.org/abs/2405.19308

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