

Future Prospects for Data-Driven Methods in Materials Science

Outline

I. OUTLINE

- Framing AM as a sub-field of materials science: other fields have tackled similar problems
 - High-throughput studies have long been used in materials science [?]
 - Multi-scale modeling has also been around in materials for a while [?]
 - Machine learning has been adopted in materials recently
 - **AM users do not need to reinvent the wheel (completely) when adopting data-driven methods for AM; they need to look to previous investigations in materials science**
- Data driven/machine learning has been picking up in materials
 - Promoted by materials genome initiative [?]
 - Examples: Photovoltaic materials [?]; Dielectric Materials [?]; Molecule Design [?]; [?]
 - Adoption of machine learning in AM should take into consideration how other fields are using it **so that standard applications of ML in materials science can be developed**
 - Review articles of ML for mat sci: [? ? ? ?]
 - **The AM field, along with other fields of mat sci, should evolve toward standard practices in the use of machine learning**
 - Maybe a good place to talk about standard data formats (e.g. the PIF)
 - The ‘standard’ adoption of ML (and what it would look like) is something that Branden, Brice, etc., may have insight on
- Moving AM toward a database-driven approach
 - Other fields are already adopting databases: Mat Proj [?], AFLOW [?]; OQMD
 - **Machine learning models can be improved with more data, therefore AM data should be widely & publicly accessible**
 - Discuss infrastructure necessary for use of AM databases