U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

ADVANCED MANUFACTURING OFFICE

AMO MYPP: Moving Applications of AI and ML from Materials Design and Discovery through Process Design and Development

Brian Valentine
AMO Technology Manager

July 12, 2018

AMO R&D Projects Program

- **The Program supports cross-cutting R&D in technology coming from Basic Energy Sciences**
  - Moving scientific concept to technology application
  - TRL 2 to TRL 4
  - Addressing manufacturing issues associated with energy efficiency, renewable energy technology development
  - Supporting higher technology risk than industry ordinarily would

AMO R&D Program Execution

- **Supporting competitive solicitations for new technology development**
  - Addressing manufacturing aspects of energy efficiency technology
  - Generally complementary to other EERE program office objectives
  - Some competitive solicitations specific to National Laboratories (“Lab Call”)
  - Other competitive solicitations for University, National Lab, Industry R&D partnerships
  - Numerous SBIR solicitations supported by EERE and Office of Basic Energy Sciences
  - Other initiatives such as HPC for Manufacturing
- **Manage the projects selected from the solicitations**

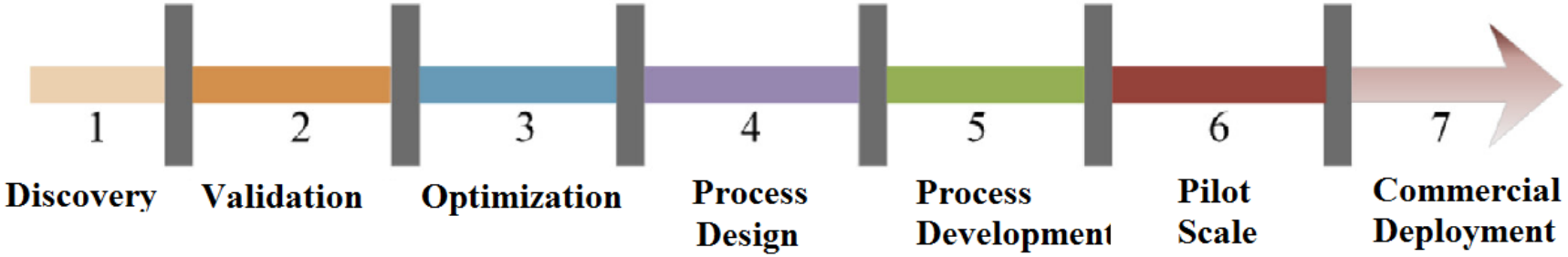
Some Materials R&D supported by the AMO Program Office

- Nanomanufacturing
- Atomically Precise Manufacturing
- Membrane development for industry, water purification
- Heterogeneous catalyst development
- New electrical conductor materials such as covetic
- Numerous other materials projects in metals, coatings, and fabrication

Goal

- **Discover and design processes for new, advanced materials required for next generation energy applications**

- **Reduce the time and costs needed to bring new energy materials to market**
  - Reduce overall material development time from 15-20 years to 3-5 years
  - Reduce development costs by 50% or more



What is the Challenge?

- **Advanced energy technologies typically require increasingly complex, advanced materials for systems and processes.**
- **Complexity is a challenge for traditional development strategies due to the extensive parameter spaces that must be explored.**
  - Development of new advanced materials from discovery to deployment typically requires two decades….
  - …But product development and manufacturing cycle has been reduced by computer-aided design to as little as 3 years.
  - RESULT: Timing mismatch prevents incorporation of new materials in products in a timely manner sacrificing both performance and competitiveness.

Solution? AI and Machine Learning

- **Artificial intelligence and machine learning (AI/ML) is a collection of methods to:**
  - Analyze vast amounts of data quickly
  - Project possible (or probable) functions of materials.
- **The methods can also be used to:**
  - Reduce the amount of calculation used in materials property simulations
  - Interpret the validity (or quality) of calculated or measured data
  - Suggest new lines of research based on possible causes with unknown effects.
- **RESULT: Tools based on AI/ML methods can expedite materials discovery by integrating synthesis, characterization, and modeling of complex materials and chemical processes and reduce design and development costs.**

Current Situation (cont.)

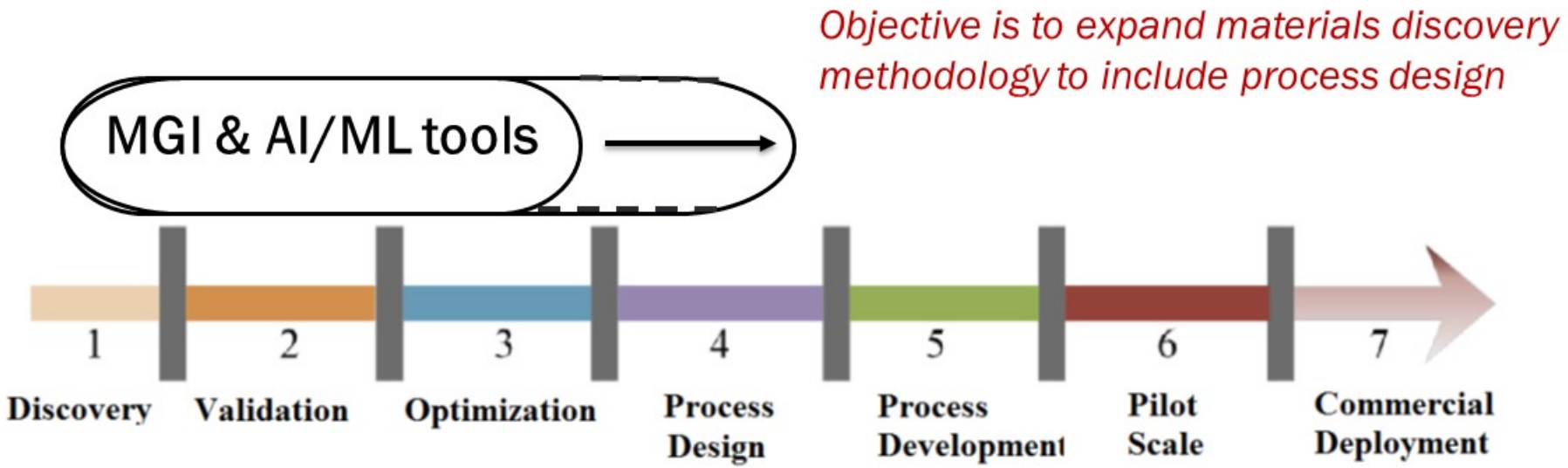
- **Materials Genome Initiative (MGI) launched in 2011 supporting efforts throughout the Federal government to accelerate materials discovery and design.**
- **MGI has provided infrastructure and training to stakeholders for advanced materials *discovery***
- **Federal government has invested in:**
  - Materials design programs supported by NSF, NIST, DOD, DOE BES
  - World-leading materials characterization tools in spectroscopy, microscopy, etc.
  - Nanoscale Science technologies in fabrication and measurement
  - Computational Facilities at the National Laboratories
- **MGI has accelerated materials discovery; MGI has not considered materials processing and manufacturing**

Challenges to Applying AI and Machine Learning to Materials Development

- Required AI/ML techniques are mostly new to industry
- Multi-disciplinary nature of AI applied to materials discovery is also difficult for companies to address due to lack of in-house expertise
- Barriers to wider industrial participation include access to data, infrastructure, and AI/ML tools
- Addressing entire materials problem, from discovery to design, processing, and manufacturing remains a challenge.

Bridging MGI with AI

- Materials Genome Initiative (MGI) is a government led effort to discover and optimize new materials for higher performance and advanced products



Opportunities to Apply AI/ML in Advanced Materials

- **Energy Generation – Photovoltaics**
  - Materials innovation in light absorbers and electrical contacts could provide increased efficiency, less cost and improved reliability while also using scalable manufacturing processes and non-critical elements.
    - Process-dependent defects and microstructure control the lifetime of photo-excited charge carriers.
- **Energy Conversion – Thermoelectrics**
  - Higher efficiency thermoelectric materials could enable practical waste heat recovery; commercially available devices are only about 5% efficient
- **Energy Storage – Battery materials**
  - Molecular formulations beyond Li-ion technologies are needed; and Li ion cathodes and electrolytes are far from optimized

What Advanced Energy Materials Are Needed?

- **Other Advanced Energy Materials**
  - Materials for harsh service conditions for use in high temperature/high pressure/corrosive regimes.
  - Heterogeneous chemical oxidation catalysts enabling direct oxidation of hydrocarbons
  - Material substitutes for Dy and Tb in Nd permanent magnets

Why DOE?

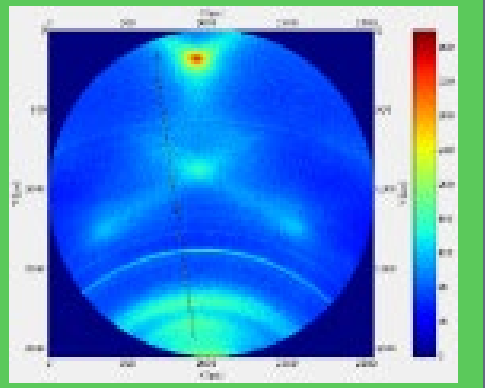
- AI and ML tools and techniques are frequently applied in specific ways to materials discovery and design problems but these methods tend to be specialized and not useful for process design
- AI and ML have not been applied to materials processing and manufacturing considerations - which determines ultimate product manufacturing potential
- This suggests the need for a unified framework of approaches that would be useful across broad areas and useful to investigators not specialized in particular techniques
- Broad energy materials development challenges that encourage collaboration would help to unify approaches to make the techniques accessible to many other potential users

Conclusions

- AI and ML have an important role in materials research to accelerate product design and processing
- MGI has added capacity in materials databases and ML-based methodologies; does not consider materials processing
- Challenges in energy materials design and processing can be addressed through inter-agency partnerships

Questions??

Advanced Energy Materials?



Describe the steps involved in applying AI and ML to materials design

- ***Goal + Sample + Algorithm = Model -> Model Evaluation***
- *Goal* – The problem to be addressed, expressed as the objective function of a targeted material property
- *Sample* – Data processing, data cleaning, feature selection, feature learning. Data can be experimental or computational.
- *Algorithm* – Learning methods such as artificial neural networks and deep learning applied to data - including regression, probability estimation, optimization.
- *Model Evaluation* – Testing of model on data not used to build model. This step can assess whether targeted material properties were under or over constrained by data used to build the model (Effects not related to possible causes or incomplete set of causes related to effects)