U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

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Summary of Findings: 2017 DOE Workshop on Artificial Intelligence Applied to Materials Discovery and Design

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Workshop on AI applied to Materials Design

- Workshop held in Pittsburgh, August 9-10, 2017
- Complementary to an international workshop held in Mexico City in September 2017
- Over 100 in attendance – representing Industry, Small Business, Academia, Government
- Purpose was to learn needs in accelerating AI applied to materials design
- Gather expert opinion on appropriate Federal role to advance the approach

Workshop presentations

- **"Accelerated Search for Materials via Adaptive Learning,"** Turab Lookman, Physics of Condensed Matter and Complex Systems Group, Los Alamos National Laboratory
  - Developing adaptive experimental design
  - Applied to discovery of NiTi alloys with lowest thermal hysteresis
  - Approach led to discovery of new compositions with lower thermal hysteresis than training data set
- **"Analyzing Large-Scale Data to Solve Applied Problems in Materials R&D,"** Bryce Meredig, Co-founder and Chief Scientist, Citrine Informatics
  - Discussion of new learning methods to accelerate materials discovery, including an active learning method called FUELS (Forest with Uncertainty Estimates for Learning Sequentially)

Workshop presentations

- **"The Materials Genome Initiative and Artificial Intelligence,"** A. Gilad Kusne, Materials Measurement Science Division, National Institute of Standards & Technology
  - NIST is one of 10 member agencies supporting Materials Genome Initiative MGI
  - NIST supports tool development for use according to knowledge management principles:
    - **Bank it:** 'Smart' data ingestion tools and repository
    - **Share it:** Tools to automatically convert data into and out of standard formats
    - **Find it:** Search for resources via the materials resource registry
    - **Check it:** Use probabilistic models to assess uncertainty (e.g., confidence, or credible intervals)
  - NIST also supports the creation of a High-throughput Experimental Materials Collaboratory (HTEMC)

Industry presentation

- **“Accelerated Materials Design and Discovery: An Industry-University Collaboration,” Brian Storey, Program Officer, Accelerated Materials Design and Discovery, Toyota Research Institute**
  - Toyota Research Institute (TRI) Mission: improve the quality of human life by pushing the boundaries of what AI can do
  - In materials research, TRI is applying AI to the discovery and development of fuel cell catalysts and polymers
  - Dr. Storey reminded us that a compound is not a material (an early criticism of MGI) and
  - a material is not a system.

INDUSTRY PANEL DISCUSSION: Challenges Facing AI in Applied Materials Design

- **William Peter (Moderator), Director, Manufacturing Demonstration Facility (MDF), Oak Ridge National Laboratory (ORNL)**
  - The MDF hosts about 700 industry customers per year
  - AI might provide insight to decide what materials system should be used for a particular application; what process and process parameters should be used to develop and design a desired part; and a high level understanding of expected performance of the desired part
- **Joe Vinciquerra, Technology Platform Leader, Additive Materials, General Electric Global Research (GEGR)**
  - Additive manufacturing technology within GEGR is accelerating rapidly
  - Biggest challenge to wider industry adoption of additive manufacturing is the slow pace of materials development

INDUSTRY PANEL DISCUSSION: Challenges Facing AI in Applied Materials Design

- **Amra Peles, Project Leader, Design for Sustainability, Pratt & Whitney**
  - Pratt & Whitney is also investing in additive manufacturing, using modeling and experimentation to apply AI-based tools to help guide development
  - Recognition of the limitations of AI-based approaches, for example, some predicted materials lie outside the domain of physical law
  - Need to design processes to rapidly scale material
- **Kishore Reddy, Staff Research Scientist/Engineer, United Technologies Research Center (UTRC)**
  - UTRC learned that strong interactions between business units and researchers during the development of AI-based tools enhances understanding and acceptance of those tools
  - There is a strong pull for service technologies from operations, manufacturing, design, maintenance, and repair – What can AI provide?

INDUSTRY PANEL DISCUSSION: Challenges Facing AI in Applied Materials Design

- **Adama Tandia**, Research Associate, Corning Incorporated
  - Corning researchers began to explore ML-based tools and techniques in 2007
  - It used to require almost two years and several million dollars to design new glass compositions
  - Researchers can now identify a selection of optimized glasses in a week
  - Coring is interested in applying AI tools to minimize glass defects. A key challenge is to develop a model that can accept an enormous amount of data and variables and provide a response in a fraction of a second.

Workshop Breakout Sessions

- **Breakout sessions addressed three focus topics**
  - Data Quantity and Quality
  - Platforms and Infrastructure
  - Collaboration, Partnerships, and Education/Training (Applications)
- **Breakout groups each responded to two or three topical questions**
- **Responses to questions were solicited and answers were collected, and voted according to importance to participants**

Workshop Breakout Session

- **Data Quantity and Quality Breakout Session - Future Capabilities and Targets**
  - **FOCUS QUESTION 1:** *What are the key capabilities, technologies, characteristics, or targets you want to see in future for AI as applied to materials discovery and design?*
    - FAIR (Findable, Accessible, Interoperable, Reusable)
    - Data Visualization Needs
    - Data Quality and Completeness
    - New Targeted Databases
    - Data Acquisition
    - Standards
    - Other, such as ease of AI application, high throughput characterization tools

Workshop Breakout Session

- **Data Quantity and Quality Breakout Session - Technical and Scientific Challenges**
  - FOCUS QUESTION 2: What are the major scientific and technical challenges that limit the application of AI for materials design and discovery? What are the problems that hinder us from realizing the desired capabilities, technologies and targets identified in Session 1?
    - Data Sharing & Publication
    - Data Review & Validation
    - Data Collection & Management
    - Other, such as identification of questions that cannot be answered with AI approach

Workshop Breakout Session

- **Platforms and Infrastructure Breakout Session - Future Capabilities and Targets**
  - FOCUS QUESTION 1: *What are the key capabilities, technologies, characteristics, or targets you want to see in future for AI as applied to materials discovery and design?*
    - Data Capture & Management
    - AI System Capability
    - Data Algorithms & Models
    - AI Application Areas
    - Data Sharing & Collaboration
    - Education and Training

Workshop Breakout Session

- **Platforms and Infrastructure Breakout Session - Technical and Scientific Challenges**
  - FOCUS QUESTION 2: *What are the major scientific and technical challenges that limit the application of AI for materials design and discovery? What are the problems that hinder us from realizing the desired capabilities, technologies and targets identified in Session 1?*
    - Data/Data Acquisition/Data Management
    - Models & Tools
    - Software
    - Fundamental Science Challenges Model/Tool Development and Strategies

Workshop Breakout Session

- **Data Quantity and Quality Group – Education and Training**
  - FOCUS QUESTION 3a: *Considering the R&D needs and pathways identified, what opportunities exist for collaborative efforts with the DOE labs and industry? What types of partnerships are envisioned that would be most successful in reaching targets and goals?*
    - Collaborative Organizations and Initiatives
    - Data Sharing and Accessibility
    - Other Areas/Topics for Collaboration

Workshop Breakout Session

- **Data Quantity and Quality Group – Education and Training**
  - FOCUS QUESTION 3b: *What education and workforce challenges need to be addressed? What skillsets or disciplines need to be further developed?*
    - Curriculum Development & Academic Programs
    - Workforce Development
    - Tools and Other Resources to Address Issue