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CHALLENGING THE LIMITS SURROUNDING THE ADOPTION OF AI-GUIDED MANUFACTURING FOR MATERIALS RELIABILITY

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U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

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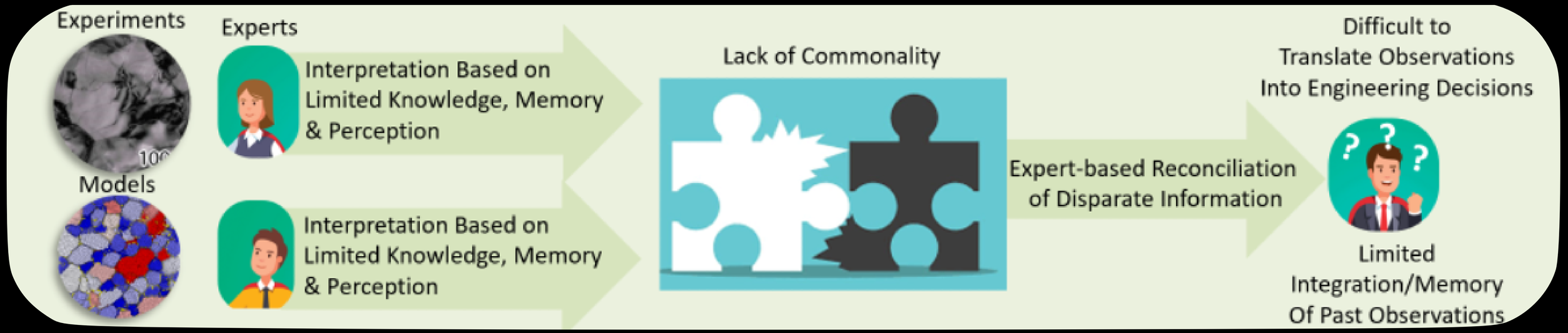
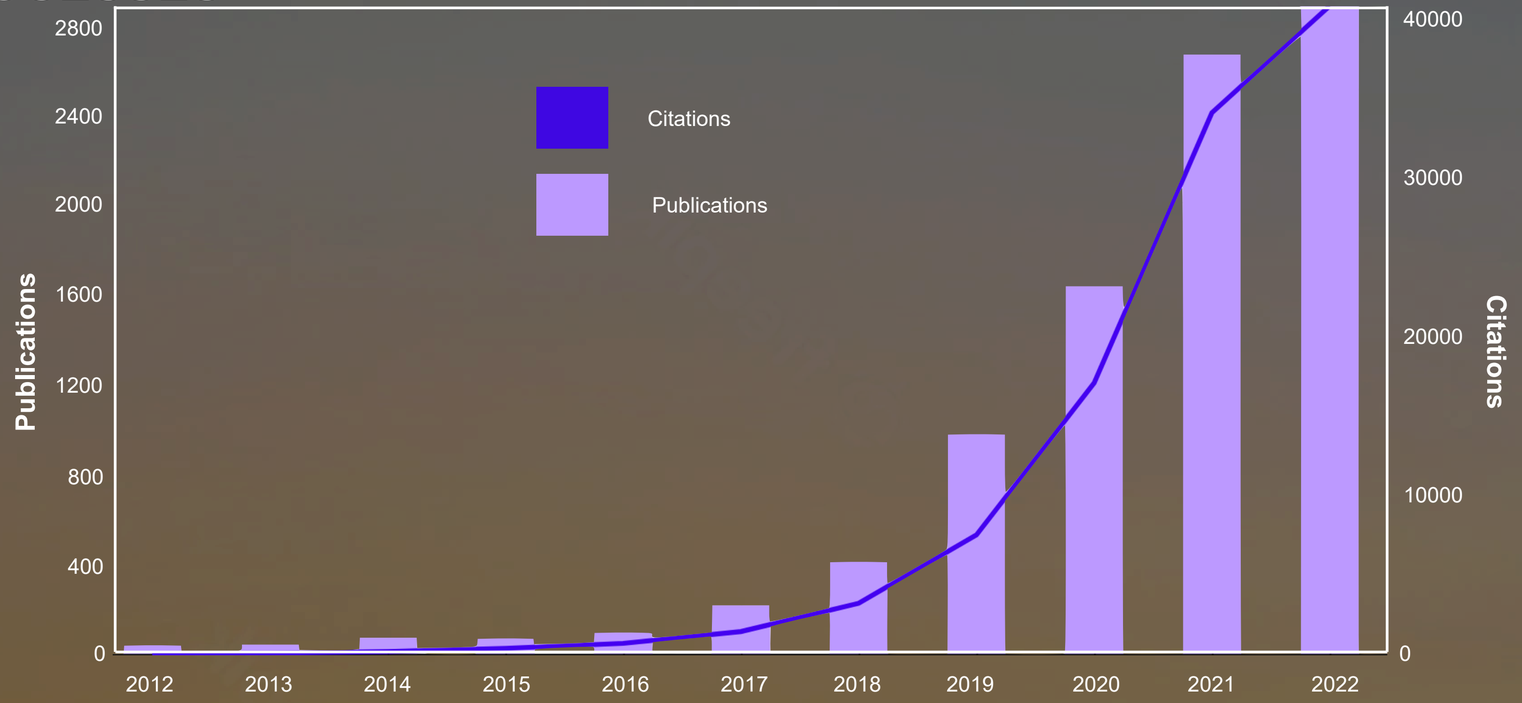
Our Current Approach to Materials Reliability is Slow, Inconsistent, Costly
and Limited by Our Own Cognition

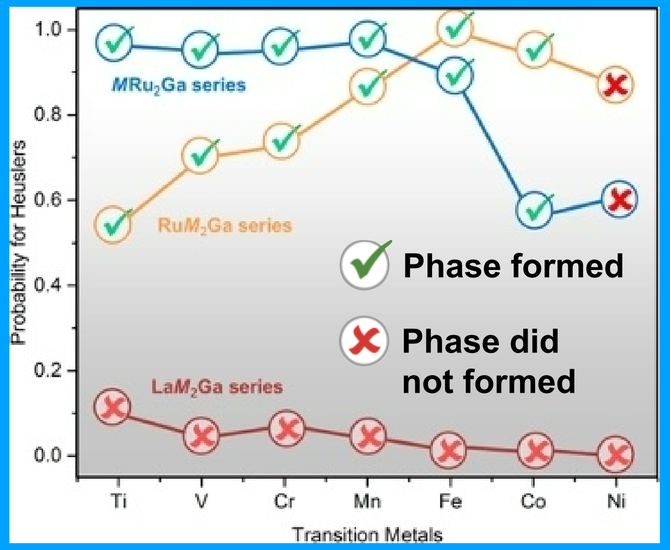


Over the Past Decade, AI has Infiltrated MSE and Manufacturing Processes



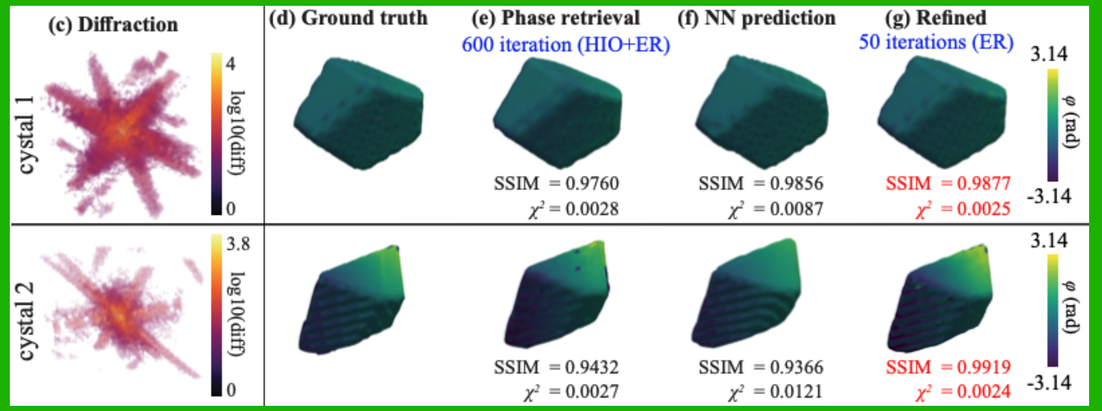
The Effective Use of AI Promises To Improve Our Ability to Do "Business" Differently

Materials Discovery



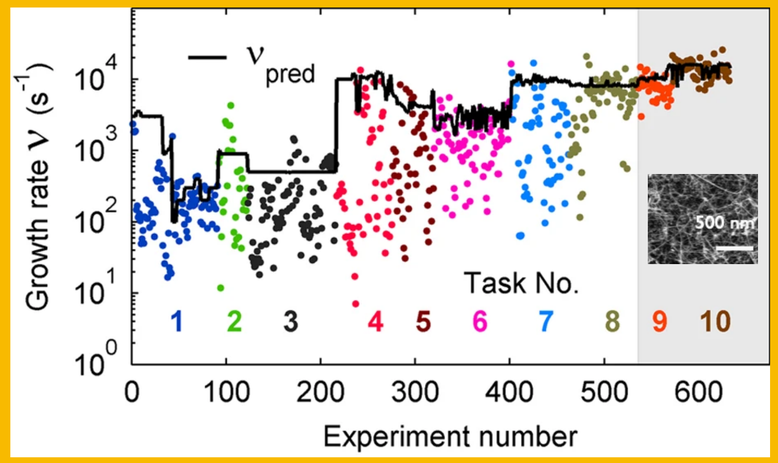
Oliynyk et al., *Chem. Mater.*, 2016

Materials Fingerprinting



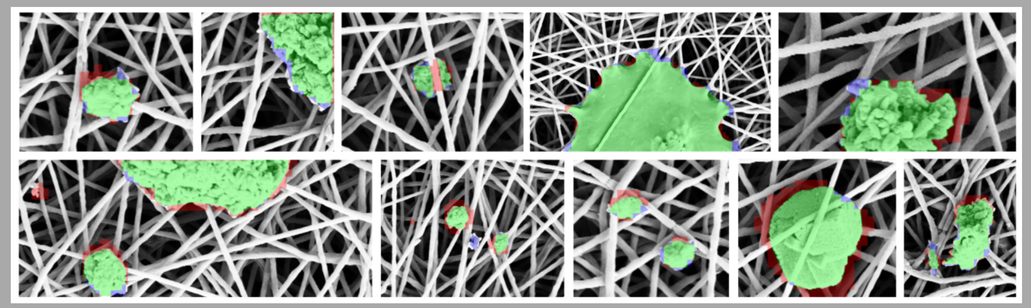
Yao et al., a*rXiv*, 2022

Autonomous Synthesis



Nikolaev et al., *npj Comput. Mater.*, 2016

Anomaly Detection



Napoletano et al., *Sensors*, 2018

Key Challenges Limiting the Integration of AI in MSE & Manufacturing…

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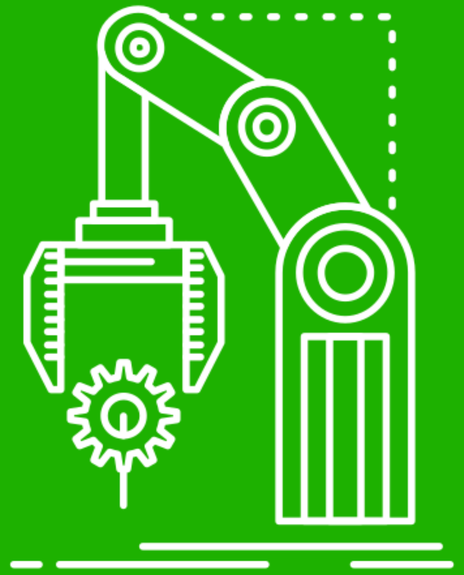
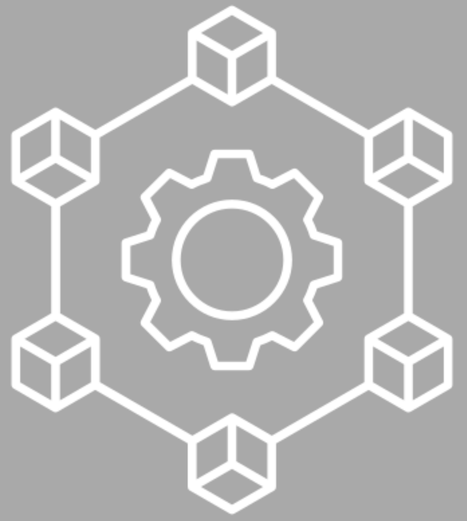
Need for greater flexibility, reliability, and trustworthiness of AI algorithms

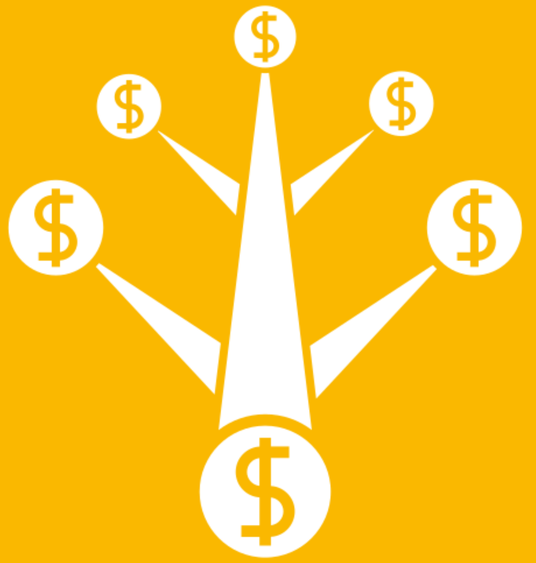
Experiments are difficult to automate



Lack of AI-related data infrastructure and best practice



Lack of large scale investments in AI for materials and materials processing



We Need to Integrate Physical Laws and Domain Knowledge By Teaching ML Models the Governing Physical Rules

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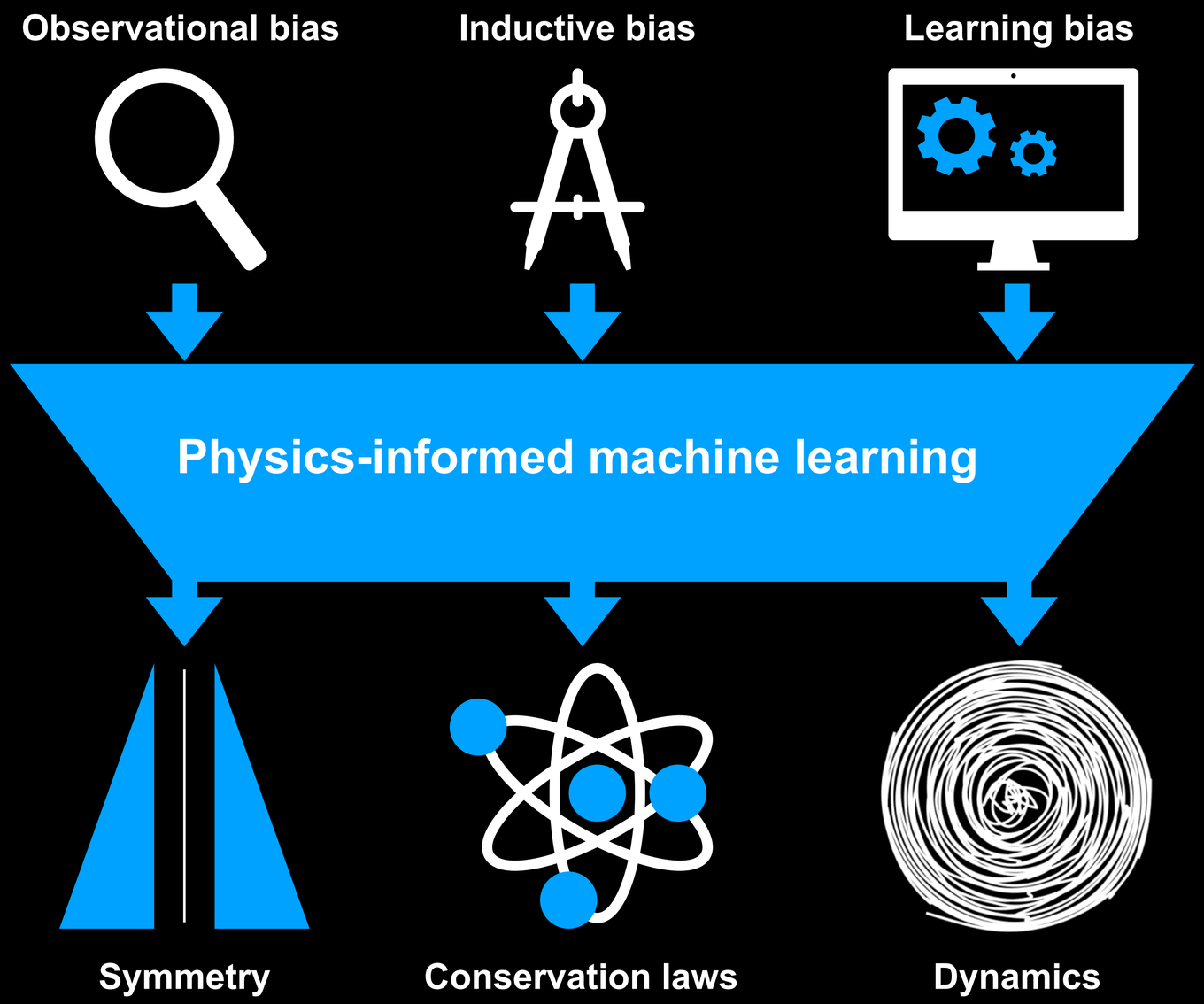
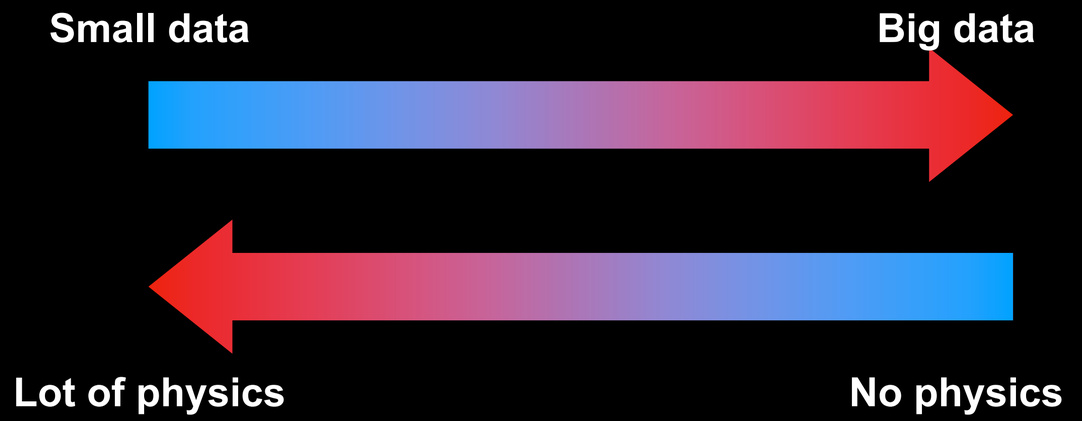
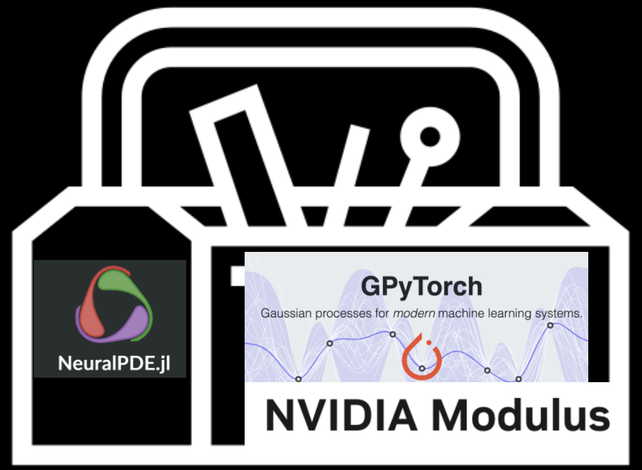




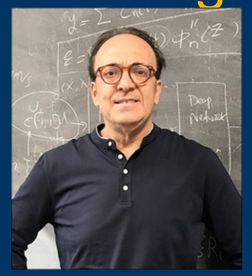


Adapted from Karniadakis et al., *Nat. Rev. Phys.*, 2022

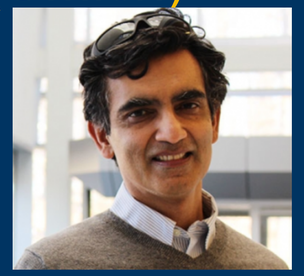
Will Physics-Informed ML Algorithms Replace SMEs?

Track for *Beyond*Fingerprinting Day 2: Wed. 9:15AM—11:30AM MT

Kardianakis (Brown), Arroyave (TAMU),
Dingreville (SNL), Martinez (SNL), Garikipati (UMich)







- Will we ever develop models that have robust extrapolation performance into untested regimes?
- Are PINNs predictions meaningless without SME or experimental validation?
- What is the path forward to develop off-the-shelf ML models that can replace known and trusted analyses and characterization capabilities?

Where Can We Replace Costly "Gold-Standard" Characterization Measurements with Low-Cost/Unconventional Methods That Contains Appropriate Signatures?

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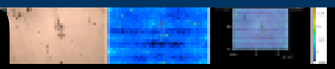
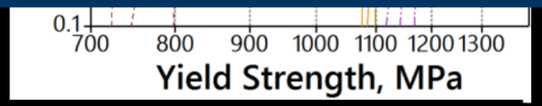
Track for *Beyond*Fingerprinting Day 2: Wed. 12:10PM—2:25PM MT

Taheri (JHU), Kalinin (UTK/Amazon),
Ophus (LBNL), Takeuchi (U Maryland), Fowler (SNL)





- Will materials scientists ever be able to trust surrogate, low-cost/unconventional measurements?
- Data-rich/data-poor dilemma: will materials science ever produce meaningful data sufficient to support AI/ML analysis?
- Will data produced by AI/ML analysis lose interpretability for SME?

Courtesy of B. Boyce for slide

Is AI/ML Algorithms and Automation All We need?

Autonomously

Track for *Beyond*Fingerprinting Day 2: Wed. 2:25PM—4:55PM MT

Hattrick-Simpers (U Toronto), Stebner (GT),
Warren (NIST), Saal (Citrine), Mehta (SLAC)





- How should we measure payoffs from ML investments, and when can we expect these payoffs to emerge?
- Will these approaches bridge from lab-scale to manufactured products with improved performance and reliability?
- Will human interpretation of ML-generated data always be a bottleneck during materials discovery?

Human Robot

Laboratories

BeyondFingerprinting Track Day 2:
AI Will Not Replace Material Scientists But Materials Scientists Who Use AI Will Replace Those Who Don't

Join us for the ***Beyond*Fingerprinting track on Day 2**
9:00AM—5:00PM MT