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Materials Design

ICME Gap Analysis in Materials Informatics: Databases, Machine Learning, and Data-Driven Design

Materials informatics is quickly becoming an essential component to materials discovery, design, and development programs. Materials informatics encompasses: (1) the collection, storage, and meaningful representation of materials data; (2) the training of models based on this data; and (3) the algorithms by which these models are used to inform materials discovery, design, and development. Although there is a growing and robust set of tools to implement and perform data-driven materials science, there are gaps and barriers to the successful integration and adoption of these tools and workflows in practice. The focus of this symposium is to evaluate performance of existing materials informatics methods for ICME and foster discussion on the challenges and future priorities of the field.

Topics include, but are not limited to:

- Comparative evaluation of materials informatics methods and tools for addressing materials design challenges
- Exploration of the limits of model interpretability and extrapolability
- Assessment of predictive capability of data-driven models and their ability to accelerate ICME workflows
- Identifying and addressing technical and cultural data-related challenges in the informatics workflow, including bias
- Materials informatics case study post-mortems, identifying lessons learned and areas for future work

ORGANIZERS

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