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Data-Driven Discovery and Property Prediction of Advanced Materials



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Data-Driven Discovery and Property Prediction of Advanced Materials

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This Special Topic welcomes contributions that integrate theory, experiment, computation, and artificial intelligence to advance materials discovery and property prediction across inorganic crystals, alloys, polymers, composites, and metamaterials.

Topics of interest

- Composition- and structure-based models for materials properties
- Graph neural networks and geometric learning
- Language, multimodal, and foundation models
- Physics-informed representations
- Transfer, few-shot, and in-context learning
- Uncertainty quantification and active learning

We particularly encourage work addressing limited or heterogeneous data, interpretability, and validation through experiments or first-principles calculations.

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Express your interest

Please contact the Guest Editors with a tentative manuscript title and proposed author list to discuss a contribution and confirm the submission arrangements.

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