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DATA-DRIVEN INVERSE MATERIALS DESIGN FOR PERFORMANCE AND SUSTAINABILITY

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ABSTRACT

Improving and accelerating materials development is a major goal in science and industry, as tailored and optimized materials are key enablers of technological innovation. Recent advances in modeling, simulation, and machine learning have brought the vision of designing materials from desired properties closer to reality. By tailoring chemical composition and microstructure, materials can be engineered to achieve specific functional and mechanical performance. Beyond performance enhancement, these capabilities also enable the development of materials that are better suited for recycling, more tolerant to contamination, and less dependent on critical or scarce raw materials, thereby contributing to a more sustainable and resilient materials economy.

This inverse design process requires computational techniques to characterize and reconstruct material microstructures and to quantify and model the behavior of phases and constituents at the microscale. Computational homogenization provides a powerful framework for linking these microstructural features to effective material properties and for understanding the mechanisms governing complex material behavior across scales.

Data analysis, machine learning, and reduced-order modeling offer new opportunities to exploit the vast amount of information generated by simulations and experiments. Surrogate models can efficiently approximate process–structure–property relationships and enable large-scale exploration of the design space. More importantly, they pave the way for true inverse design strategies, where desired material properties, performance targets, sustainability requirements, or manufacturing constraints are used as inputs to identify suitable microstructures, compositions, or processing routes.

Topics of interest covered within this mini-symposium include but are not limited to:

- techniques for exploration and inversion of process-structure-property linkages,
- microstructure characterization and reconstruction,
- inverse design approaches for micro-heterogeneous and architected materials,
- machine learning and data-driven approaches to constitutive modeling and multiscale simulations.