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Data Science Approaches for Mining Structure-Property-Processing Linkages from Large Datasets

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Materials with enhanced performance characteristics have served as critical enablers for the successful development of advanced technologies throughout human history, and have contributed immensely to the prosperity and well-being of various nations. Although the core connections between the material's internal structure (i.e. microstructure), its evolution through various manufacturing processes, and its macroscale properties (or performance characteristics) in service are widely acknowledged to exist, establishing this fundamental knowledge base has proven effort-intensive, slow, and very expensive for a number of candidate material systems being explored for advanced technology applications. It is anticipated that the multi-functional performance characteristics of a material are likely to be controlled by a relatively small number of salient features in its microstructure. However, cost-effective validated protocols do not yet exist for fast identification of these salient features and establishment of the desired core knowledge needed for the accelerated design, manufacture and deployment of new materials in advanced technologies. The main impediment arises from lack of a broadly accepted framework for a rigorous quantification of the material's internal structure, and objective (automated) identification of the salient features in the microstructure that control the properties of interest.

Materials Informatics focuses on the development of data science algorithms and computationally efficient protocols capable of mining the essential linkages in large multiscale materials datasets (both experimental and modeling), and building robust knowledge systems that can be readily accessed, searched, and shared by the broader community. Given the nature of the challenges faced in the design and manufacture of new advanced materials, this new emerging interdisciplinary field is ideally positioned to produce a major transformation in the current practices. The novel data science tools produced by this emerging field promise to significantly accelerate the design and development of new advanced materials through their increased efficacy in gleaning and blending the disparate knowledge and insights hidden in "big data" gathered from multiple sources (including both experiments and simulations). Our ongoing research has outlined a specific strategy for data science enabled development of new/improved materials, and key components of the proposed overall framework are illustrated with examples.