The objective of this PSED project is to establish a “microstructure-mediated design” approach combined with advanced data-mining techniques to facilitate the computational design of heterogeneous materials, specifically for the polymer nanodielectric material system. The capability of utilizing existing data from previous research is essential for further facilitating the design of new materials. Material informatics is such a growing area that exploits information technology and data science to represent, manage and analyze material data for accelerating the new material discovery and design. Data mining and machine learning techniques have been applied to exploit material databases and discover trends and mathematical relations for material design.

RESEARCH OBJECTIVE

Final Deliverables

- data mining tools for material design concept selection;
- interphase modeling: interphase shifting factor calibration tools and overlapped interphase models;
- microstructure reconstruction tools based on Gaussian random field (GRF) and established structure-property relationship for epoxy-silica system.