



The project includes (left) growth and characterization, (middle) iterative modeling, and (right) design training and validation. Single-frame red boxes represent experimental samples and data, while double-framed blue boxes represent computational products. The shaded region in the middle represents the application of particle swarm optimization. The general flow can be understood as: (1) growth of samples varied by composition and growth procedures; (2) experimental structural characterization; (3) iterative model simulation using characterization data; (4) ANN training to link simulation and growth parameters followed by predictive application of the ANN.