Artificial Intelligence, Al

(Generic term, mimic cognitive functions)

Machine Learning, ML

(Number of samples > 100)

Linear Regression, Random Forest, Decision Trees, Gaussian Processes, ...

Deep Learning, DL

(Number of samples > 500)

Artificial Neural Network (ANN), Convolution Neural Network (CNN), Graph Neural Network (GNN), Variational Encoders (VAE), Generative Adversarial Network (GAN), Recurrent Neural Network (RNN), Deep Reinforcement Learning (DRL), ...

Chemical Formula, SMILES, Fragments

Atomic Structure (Molecules, Solids, Proteins)

Text/Literature

XRD, XAS, Raman, NMR, UV-vis, XANES, Electron/Phonon DOS

SEM, STM, STEM images