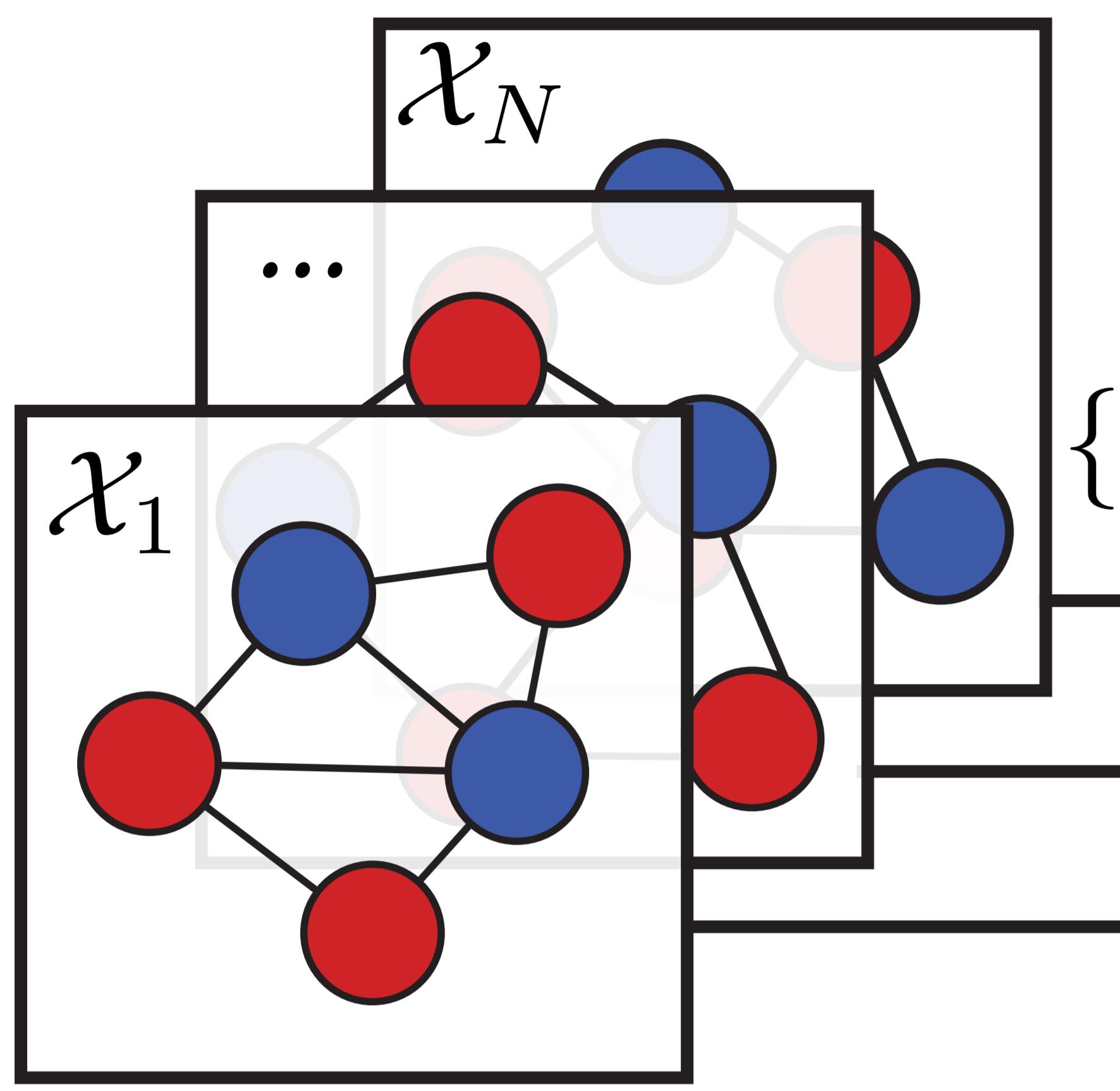
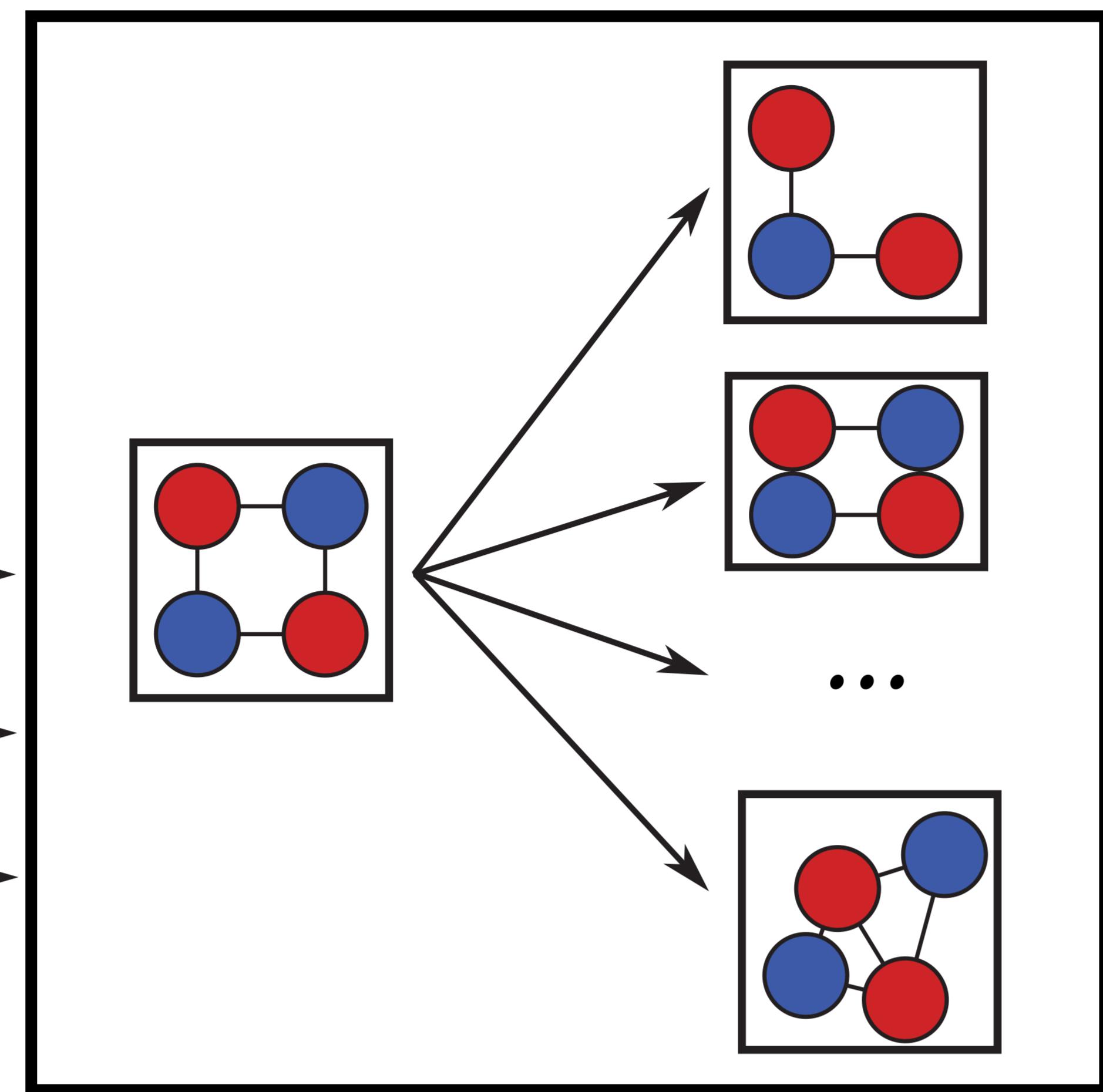


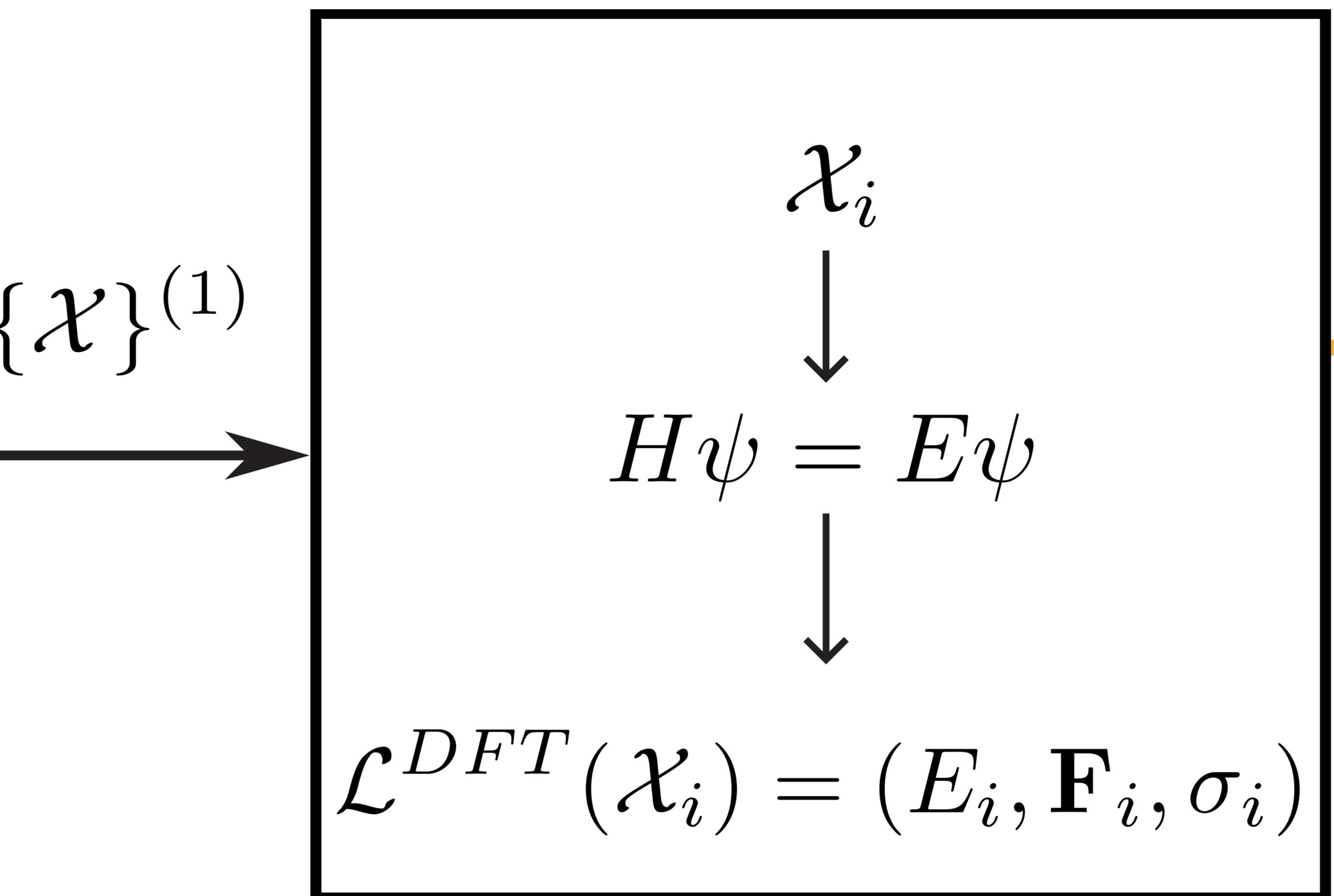
Input Structures



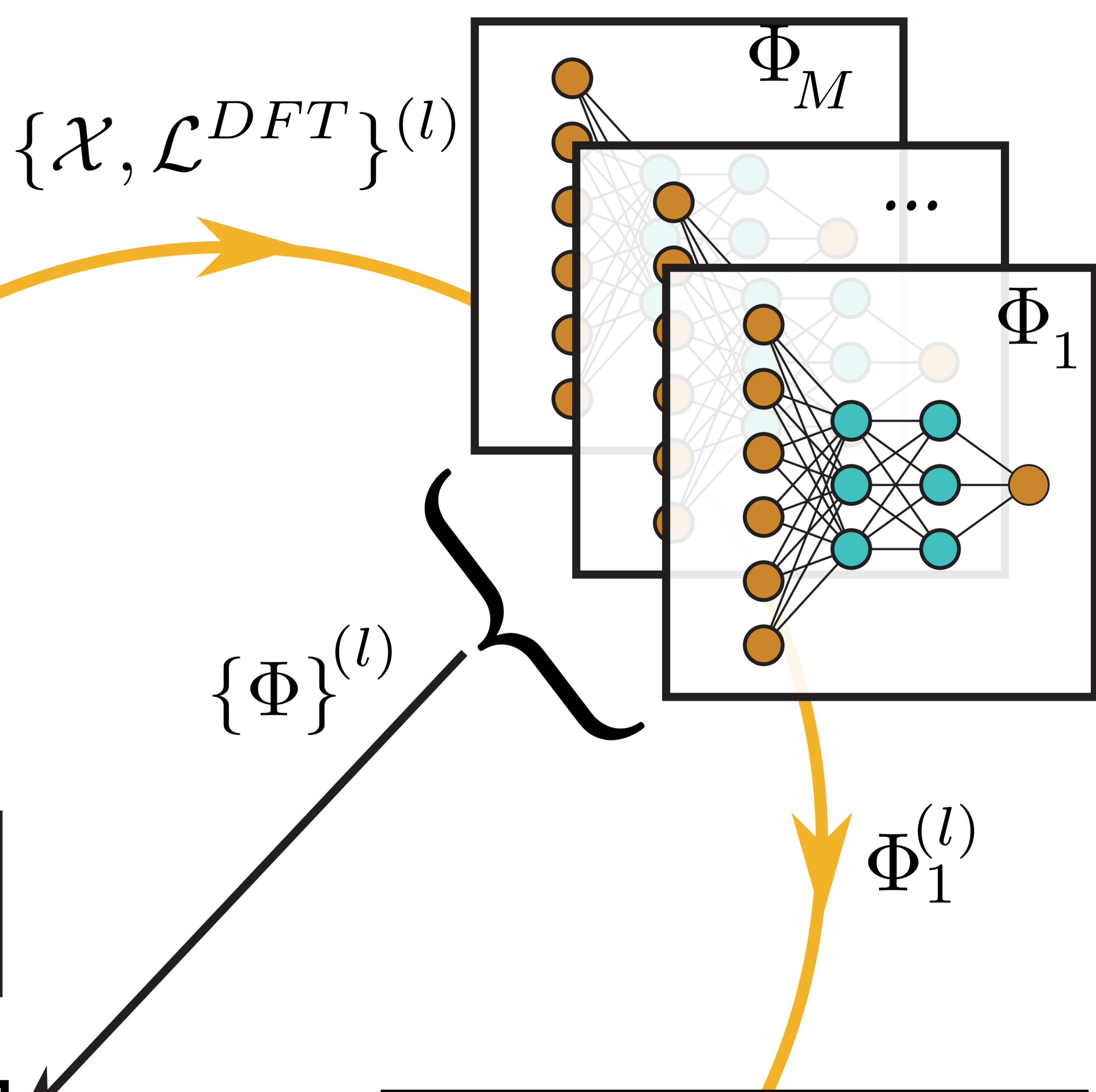
Dataset Augmentation



Ab Initio Labelling



Training



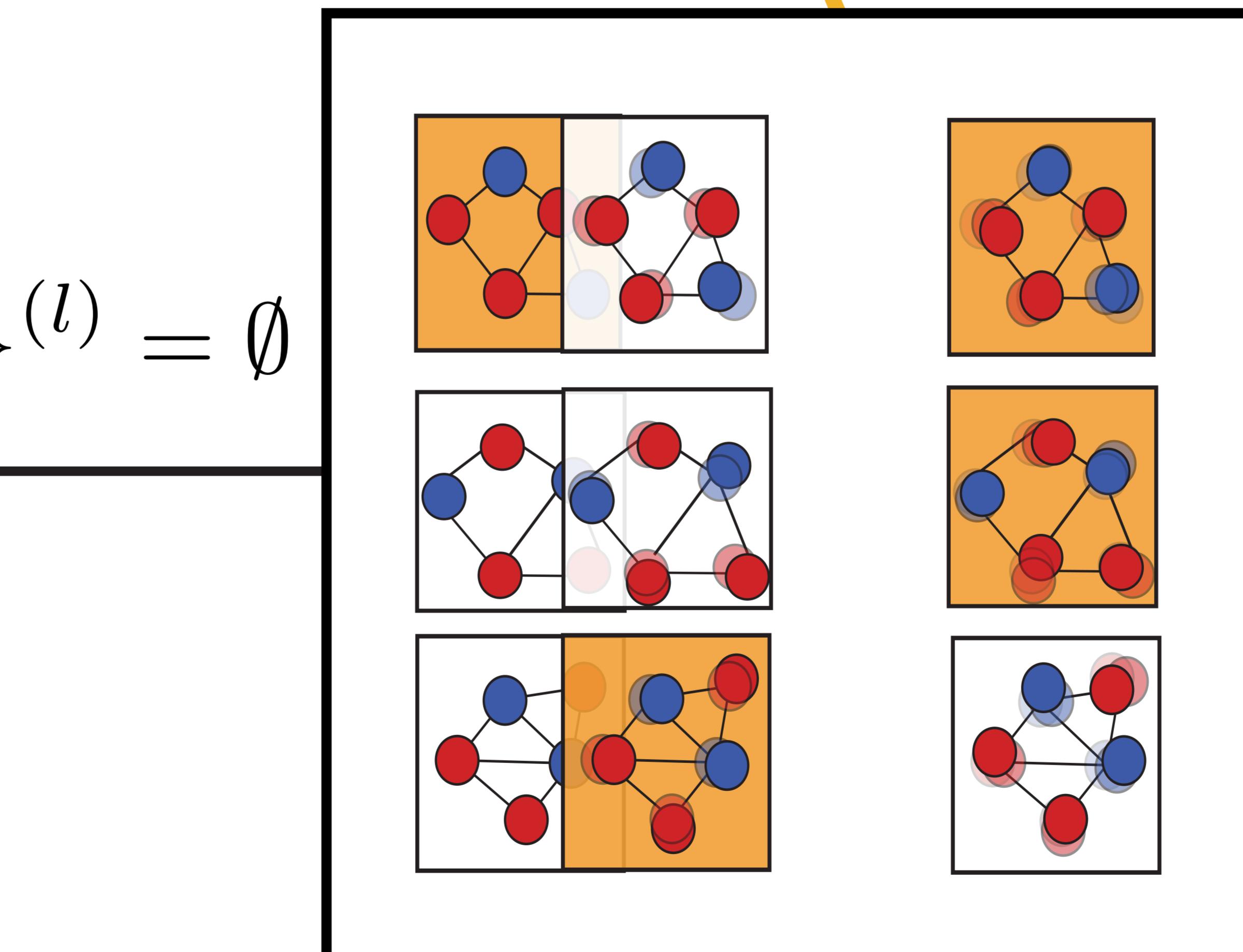
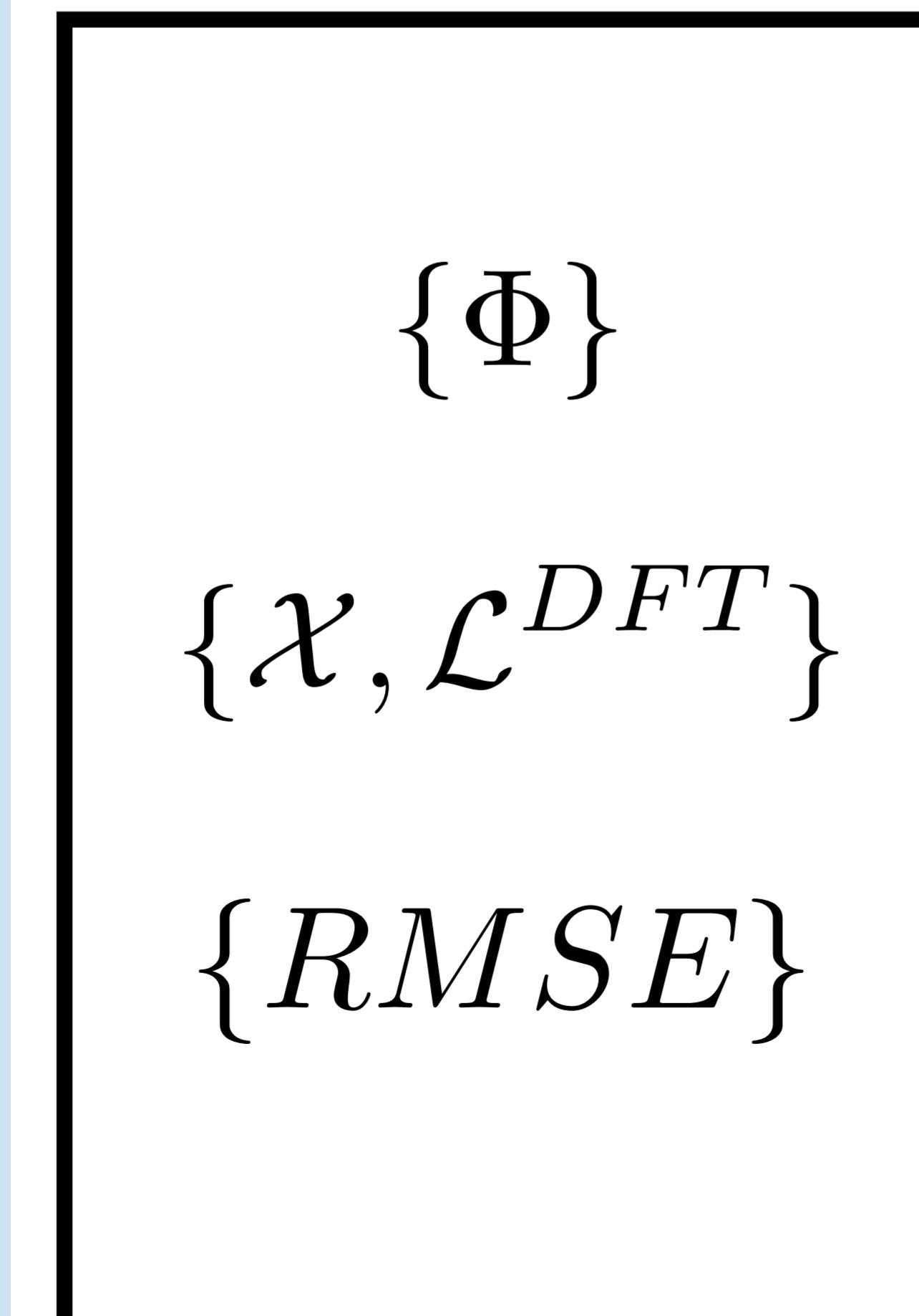
\mathcal{X} - structure information

\mathcal{L}^{DFT} - *ab initio* energies, forces and stresses tensors

Φ - interatomic potential

\mathcal{D} - calibration committee disagreement

τ^{thr} - threshold of energy, force and stress



Committee Evaluation

Exploration

