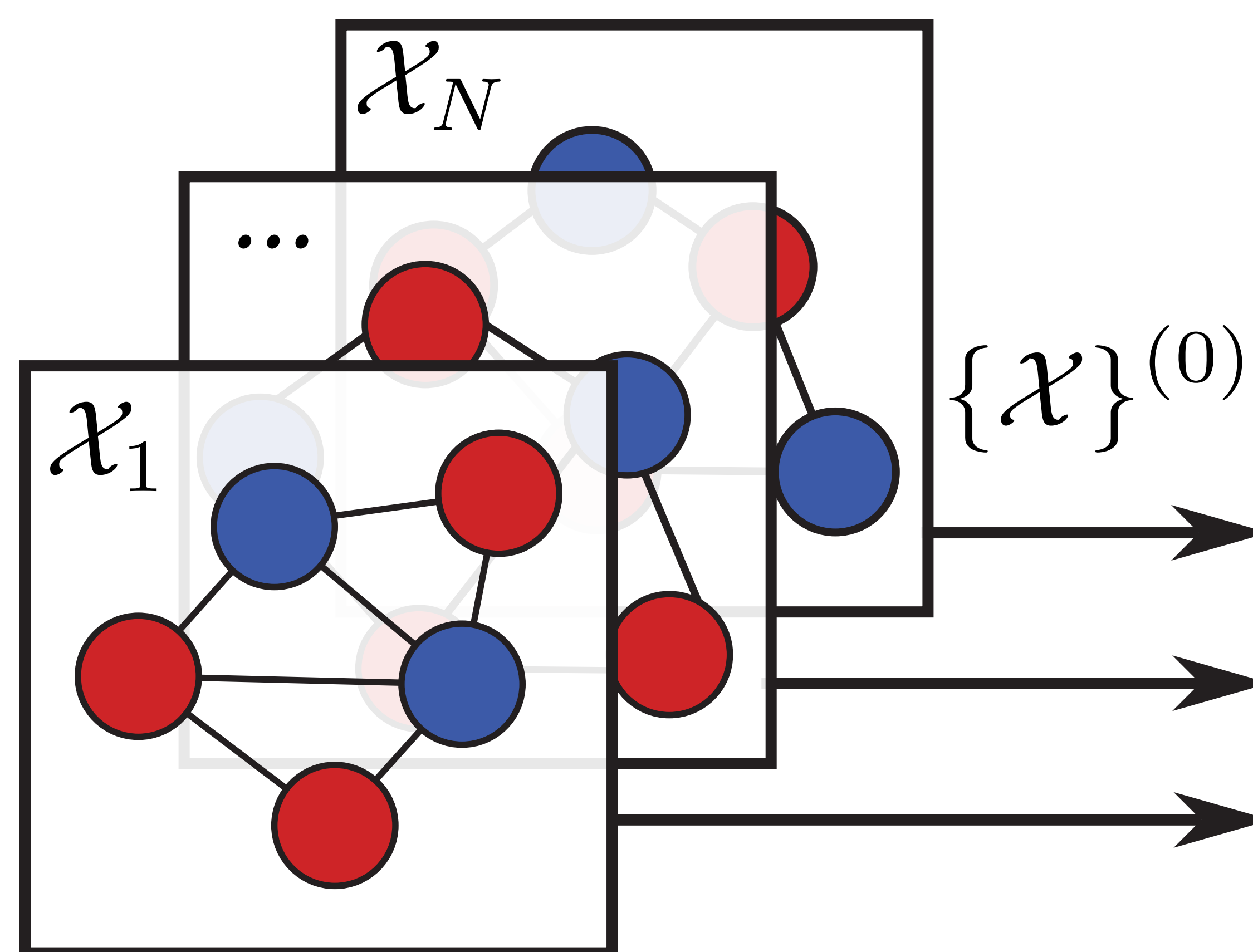
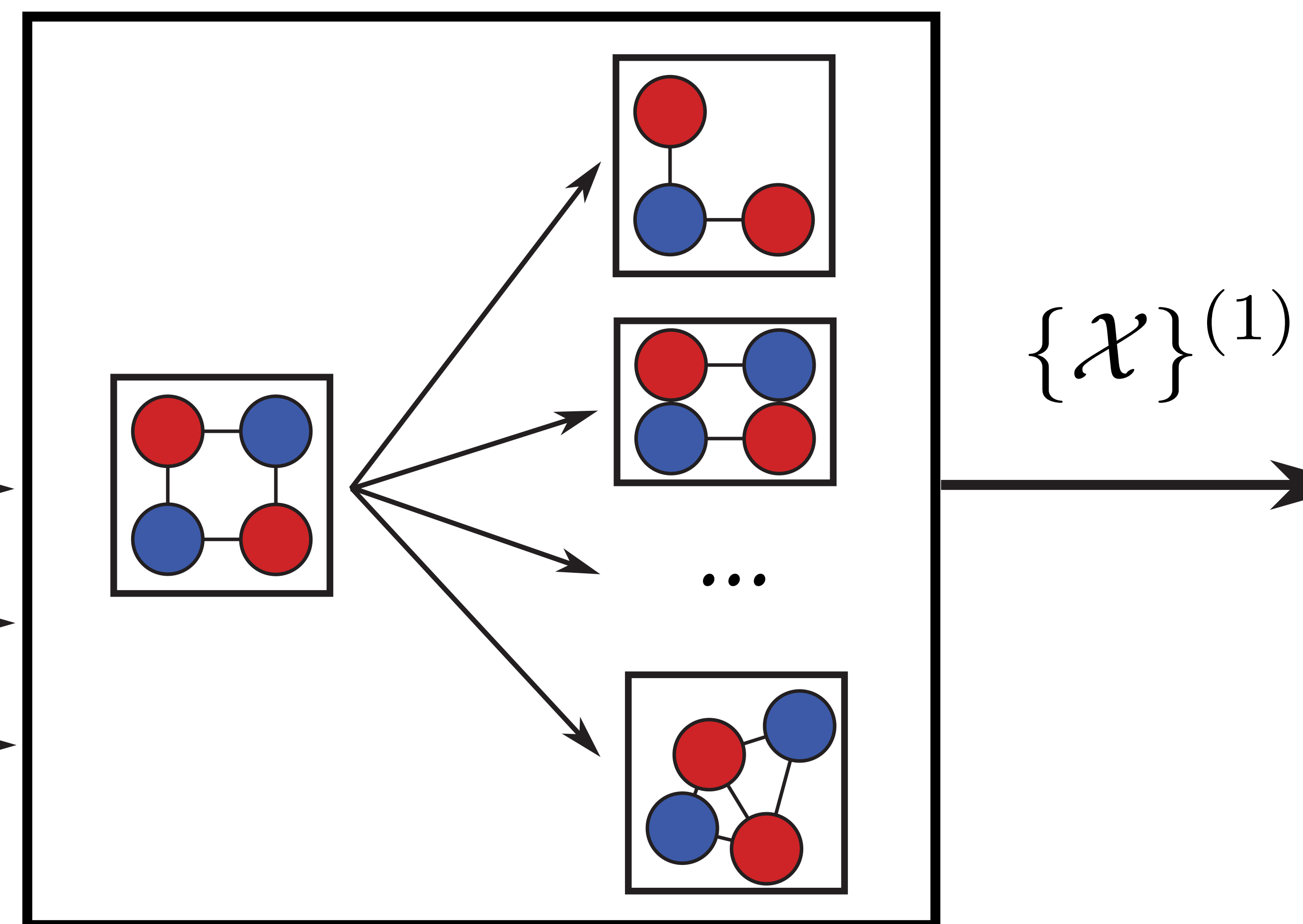


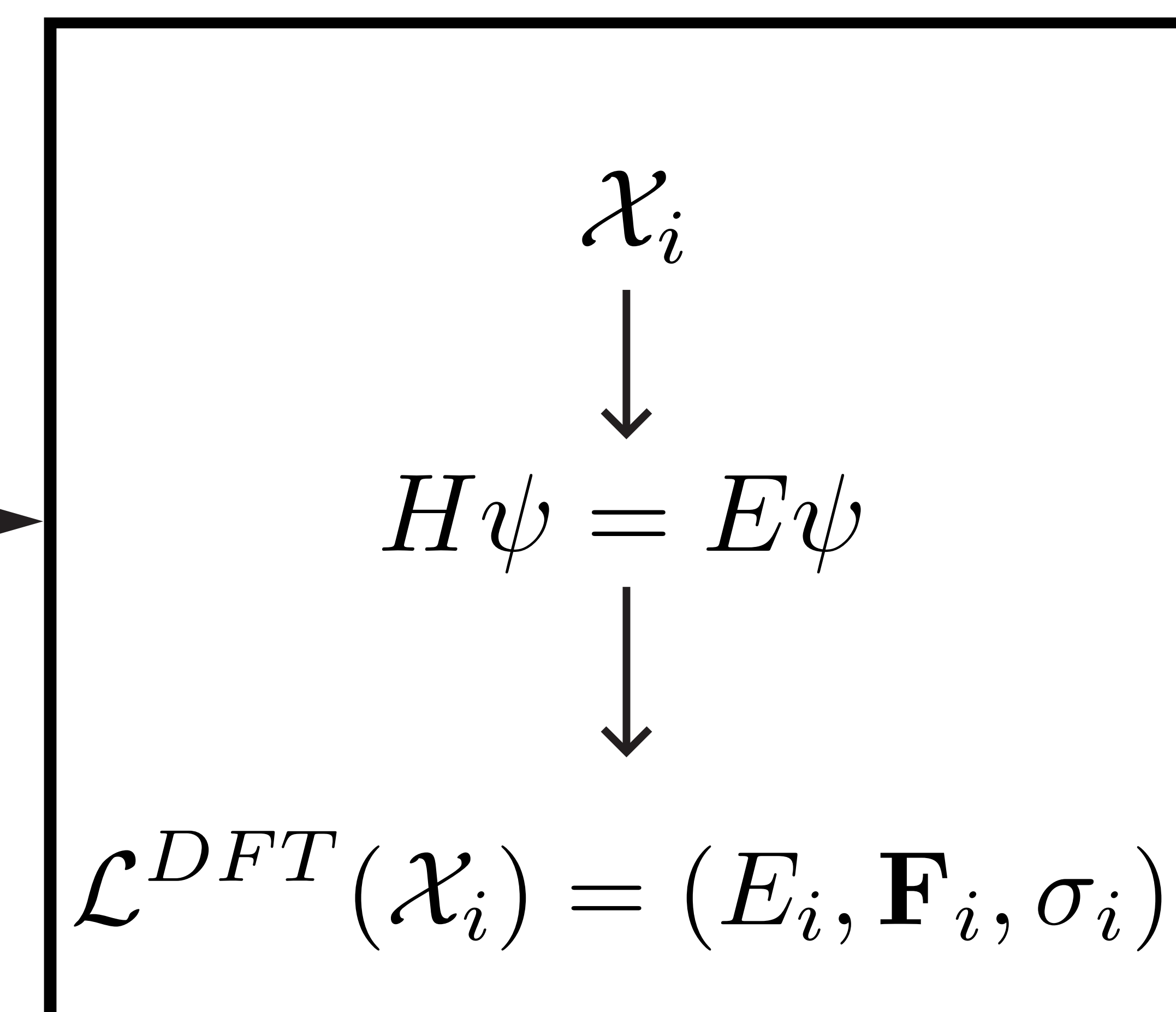
## Input Structures



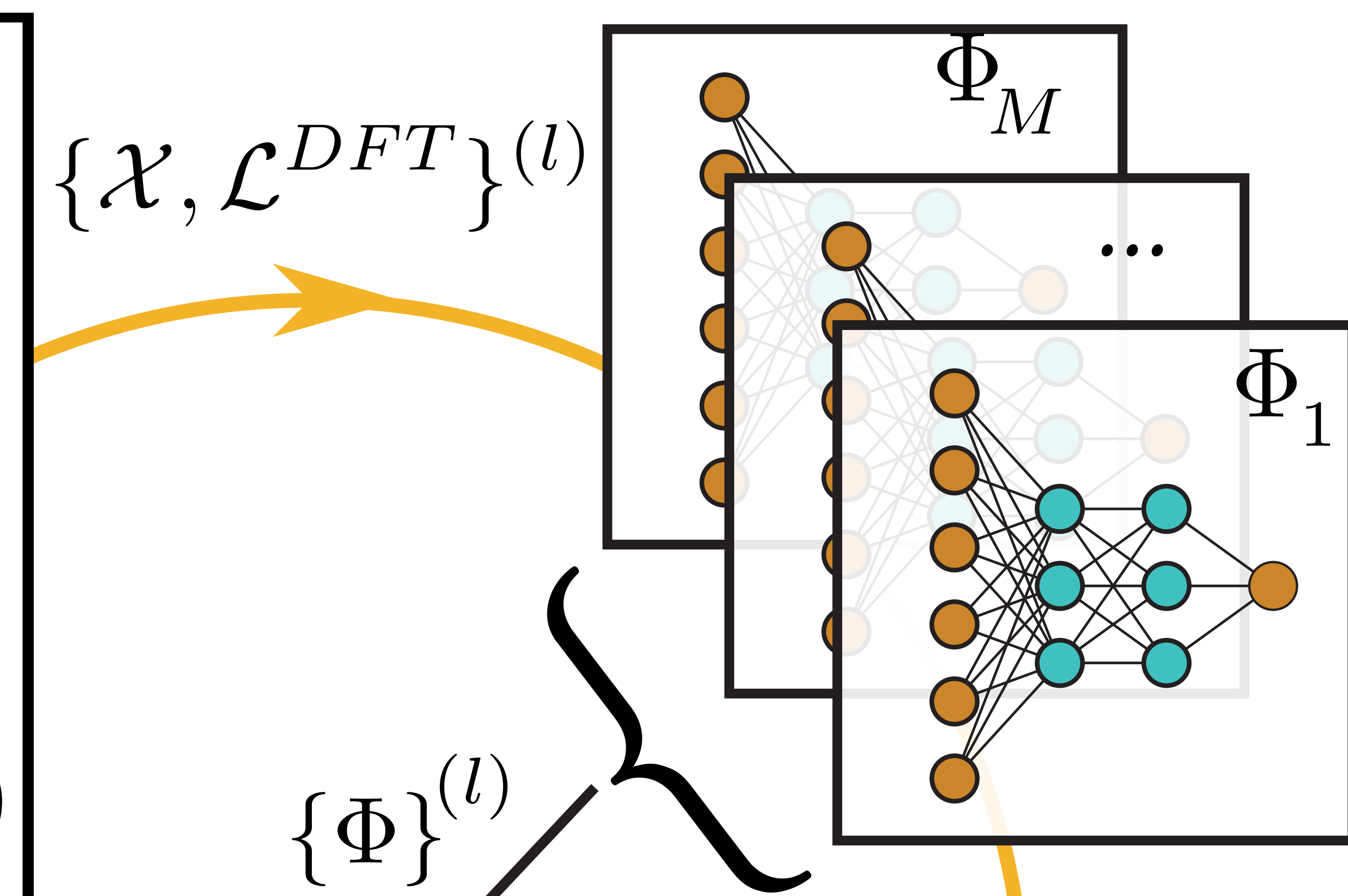
## Dataset Augmentation



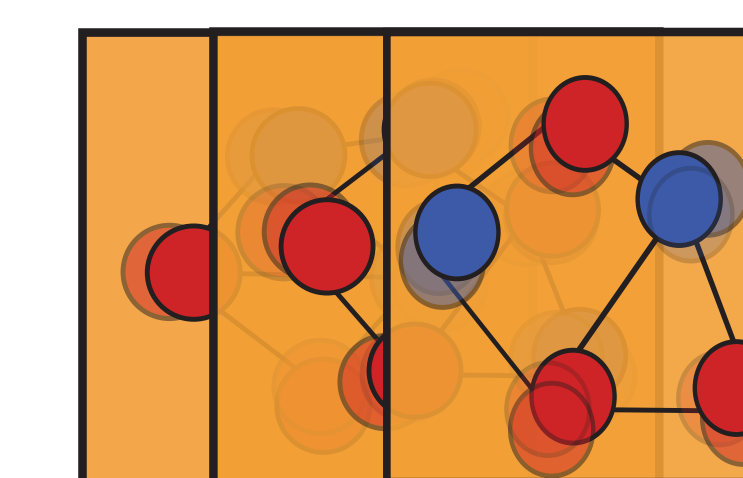
## *Ab Initio* Labelling



## Training

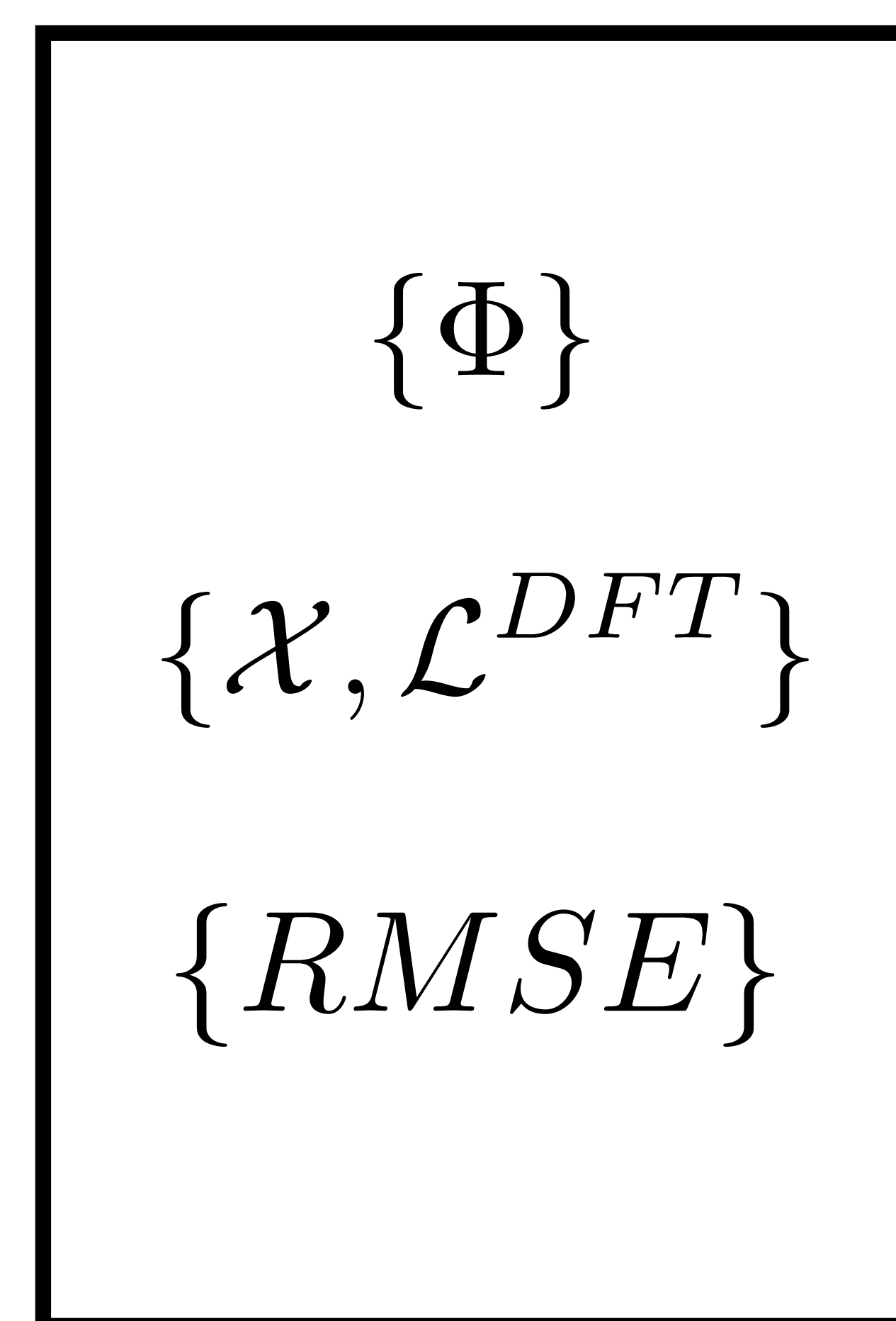


$$\{\mathcal{X} : \mathcal{D} > \tau^{thr}\}^{(l)}$$

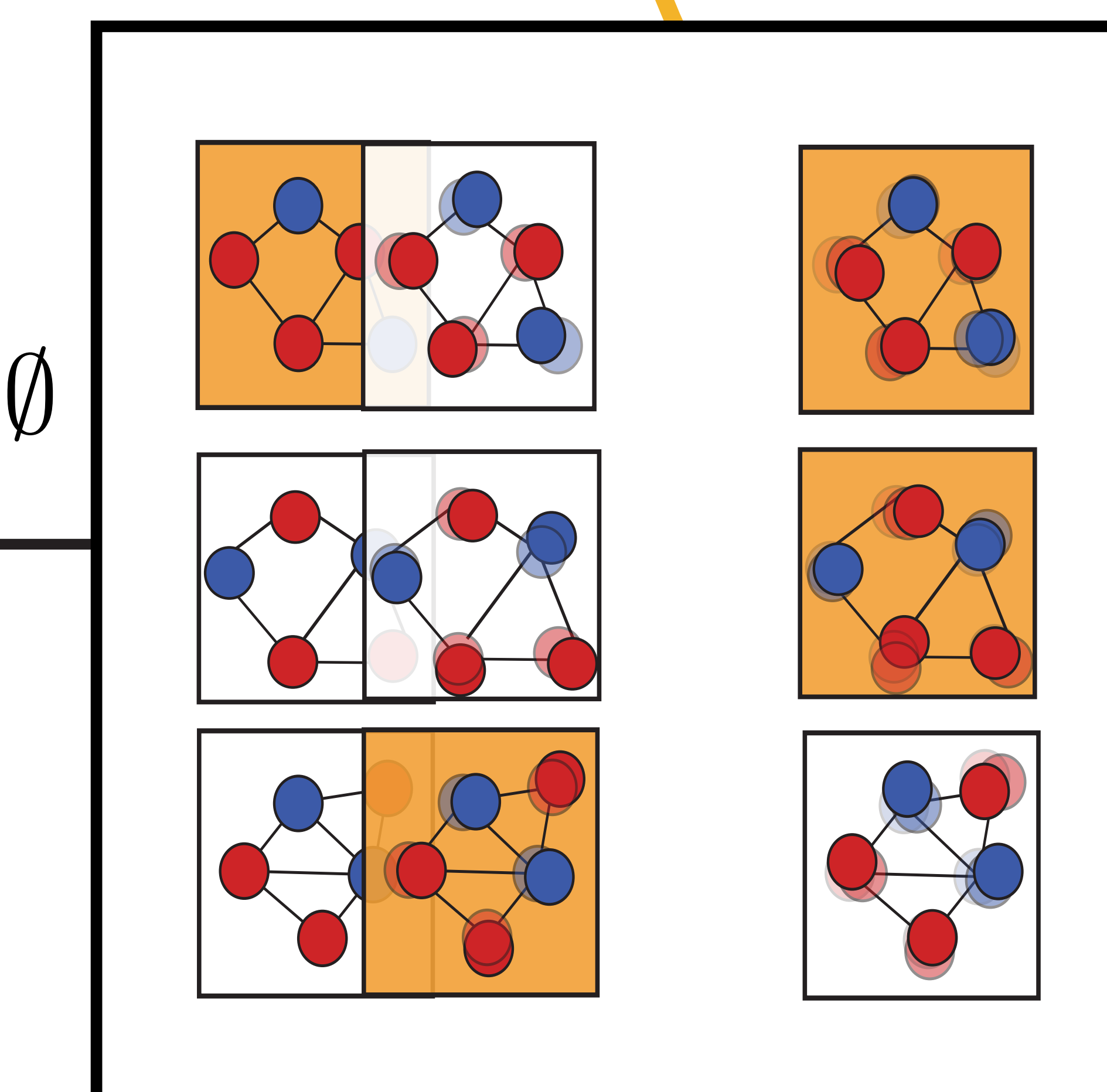


$$\Phi_1^{(l)}$$

$\mathcal{X}$  - structure information  
 $\mathcal{L}^{DFT}$  - *ab initio* energies, forces and stresses tensors  
 $\Phi$  - interatomic potential  
 $\mathcal{D}$  - calibration committee disagreement  
 $\tau^{thr}$  - threshold of energy, force and stress

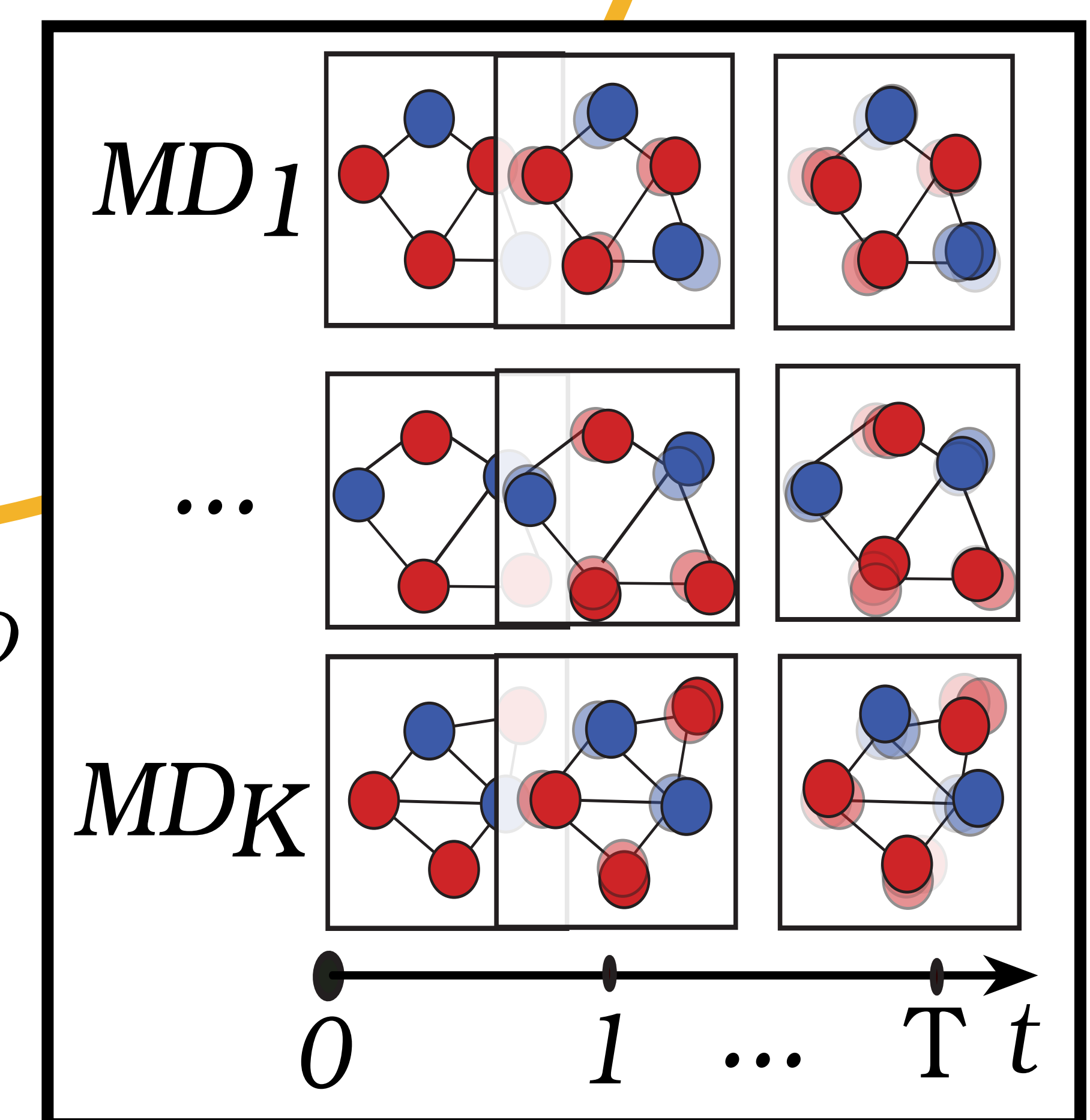


$$if \{\mathcal{X} : \mathcal{D} > \tau^{thr}\}^{(l)} = \emptyset$$



## Committee Evaluation

$$\{\mathcal{X}\}^{(l), MD}$$



## Exploration