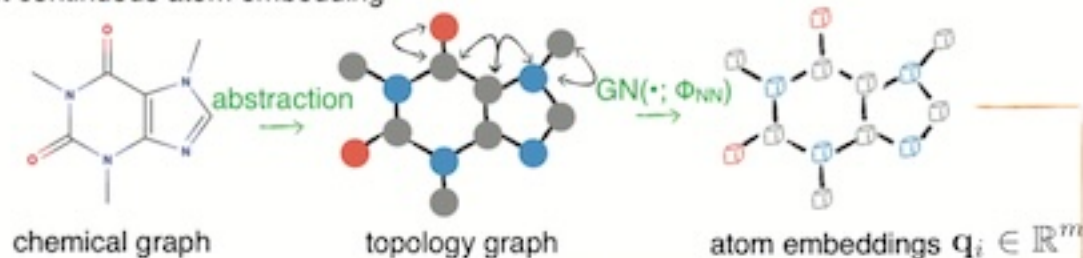
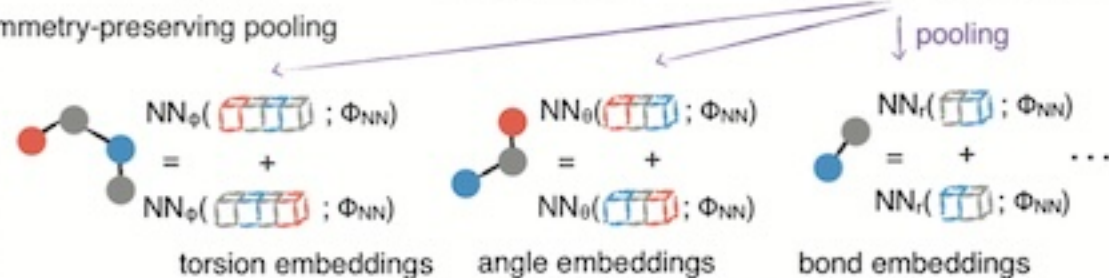


Foundation

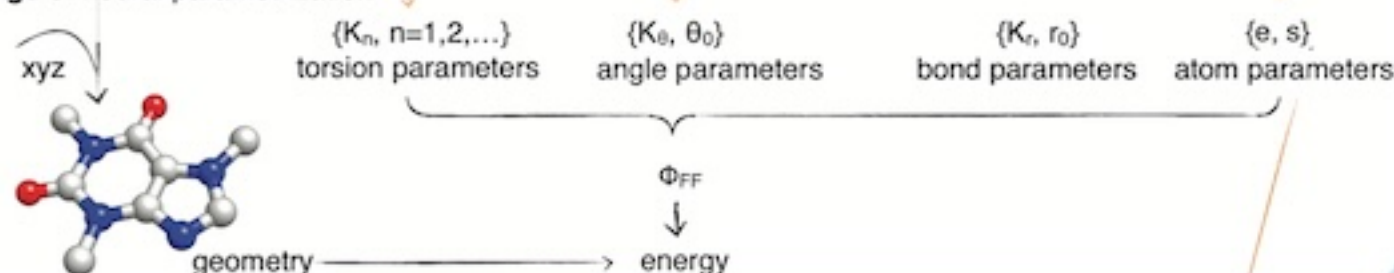
Stage 1: graph net continuous atom embedding



Stage 2: symmetry-preserving pooling



Stage 3: neural parametrization



$$\hat{q}_i^* = -e_i^* s_i^* + s_i^{*-1} \frac{Q + \sum_j e_j^* s_j^{*-1}}{\sum_j s_j^{*-1}}$$

charge
equilibration (QEq)

$$\begin{bmatrix} e_i^* \\ s_i^* \end{bmatrix} = \begin{bmatrix} e_i \\ s_i \end{bmatrix} + \begin{bmatrix} -\theta_e^T \\ -\theta_s^T \end{bmatrix} \hat{\mathbf{h}}_i$$

$\Theta_{2 \times r}$

Low-Rank Fine-Tuning

pool atom
embeddings

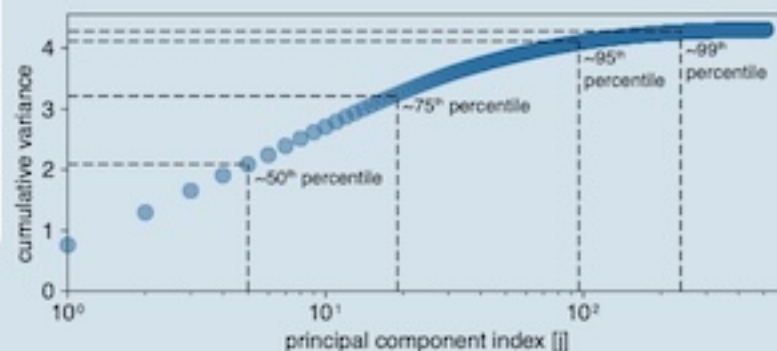
$$\mathbf{H} = [\mathbf{h}_1, \dots, \mathbf{h}_n]_{m \times n}$$

PCA, truncate covariance to r

$$\Sigma_h = (\mathbf{H} - \mu_h)_{m \times n} (\mathbf{H} - \mu_h)_{n \times m}^T \quad \mu := \text{mean}$$

$$\approx \begin{bmatrix} | & & | \\ \mathbf{q}_1 & \dots & \mathbf{q}_r \\ | & & | \end{bmatrix} \begin{bmatrix} \sigma_1^2 & & \\ & \dots & \\ & & \sigma_r^2 \end{bmatrix} \begin{bmatrix} -\mathbf{q}_1^T \\ \dots \\ -\mathbf{q}_r^T \end{bmatrix}$$

$\mathbf{Q}_{m \times r} \quad \Sigma_{r \times r} \quad \mathbf{Q}_{r \times m}^T$



change embedding basis

$$\hat{\mathbf{h}}_i = \mathbf{Q}_{r \times m}^T \mathbf{h}_i$$

compute
electrostatic
perturbations