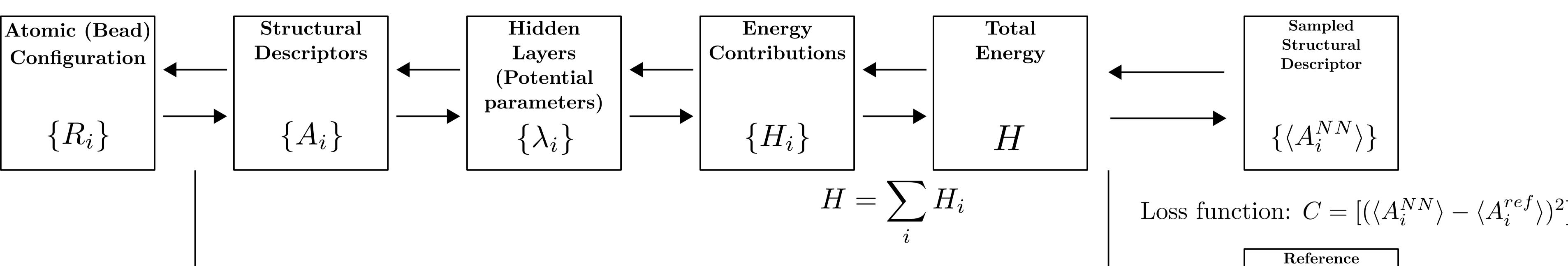
## Machine Learning Inverse Monte Carlo Algorithm

$$\frac{\partial \langle A_{\alpha} \rangle}{\partial \lambda_{\gamma}} = -\beta \left( \left\langle \frac{\partial H}{\partial \lambda_{\gamma}} A_{\alpha} \right\rangle - \left\langle \frac{\partial H}{\partial \lambda_{\gamma}} \right\rangle \langle A_{\alpha} \rangle \right)$$



Hidden Layers

Input Layer

Output Layers

Reference Structural Descriptor

 $\{\langle A_i^{ref}\rangle\}$