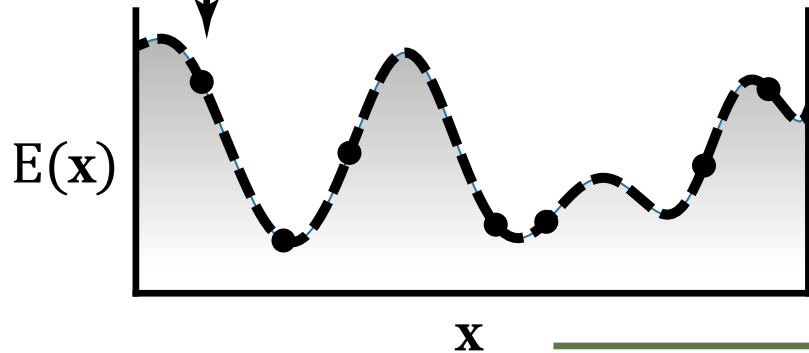
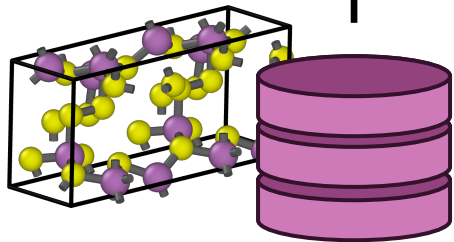
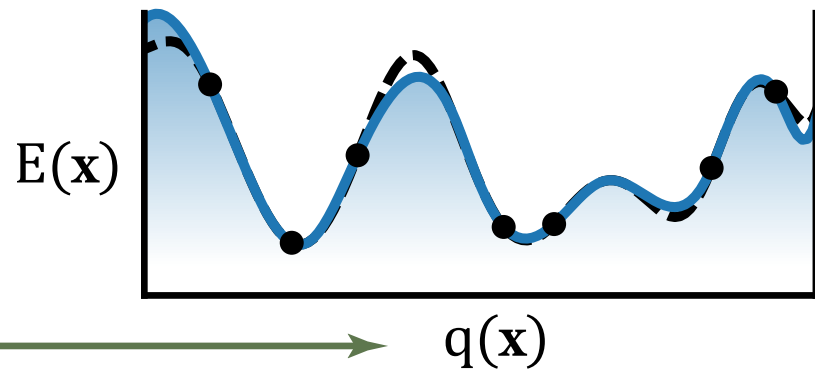


1 structures (locations) and
reference method (labels)



2 representation (e.g. SOAP)



3 regression method (e.g. GAP)

$$E_{\text{QM}} \approx \sum_i^N \tilde{\varepsilon}(\mathbf{q}_i)$$