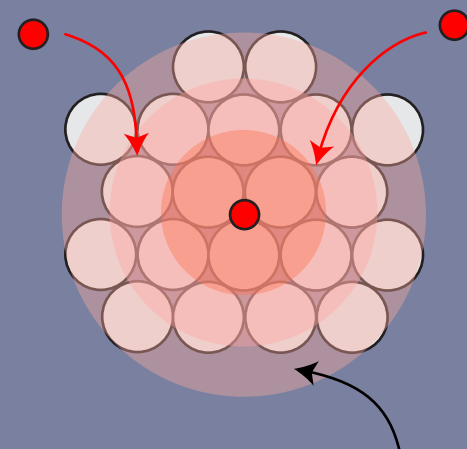
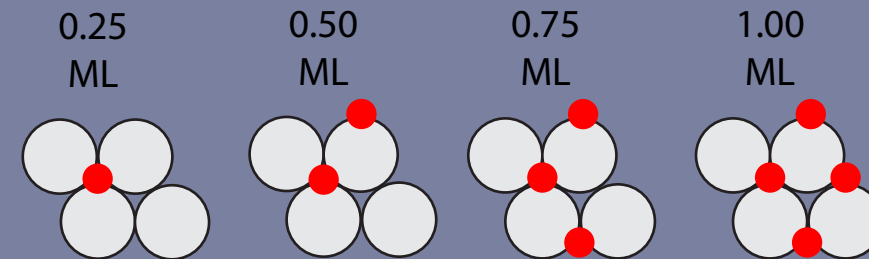


Lateral Interactions between adsorbates

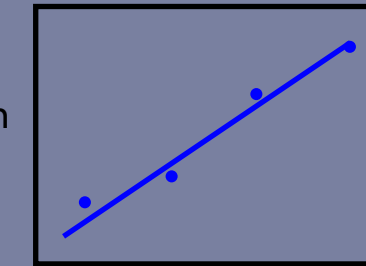


Local environment variation induced by adsorbates

Analytic linear relationships

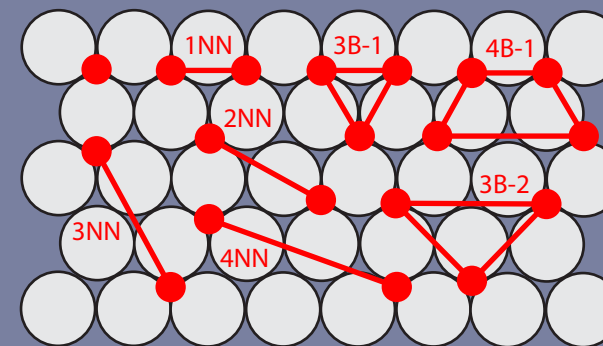


Adsorption Energy



Coverage →

ML-parameterized cluster expansions



Cross Validation

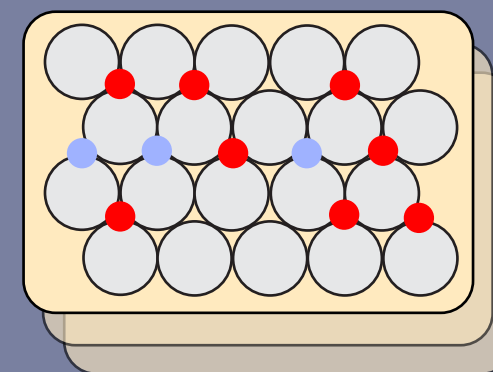
Parameterization

Regularization

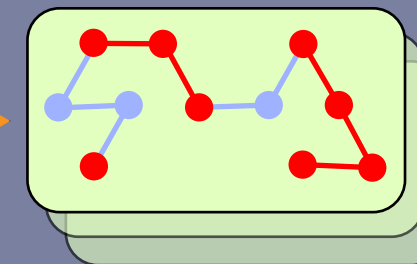
Pattern Recognition



Highly nonlinear deep learning models



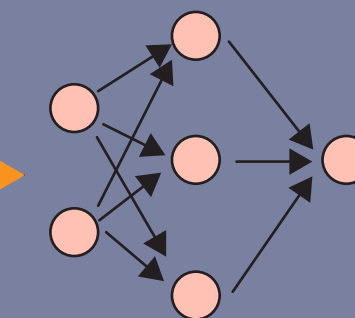
Surface configurations



Surface graph representation



Convolutional layers



Hidden layers

Output