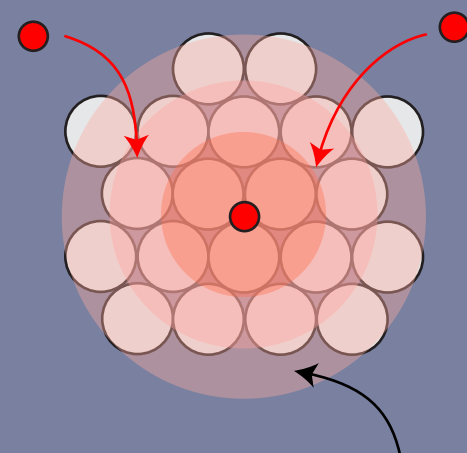**Lateral Interactions between adsorbates**
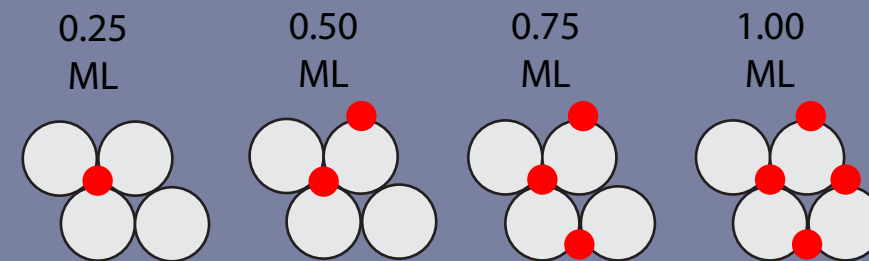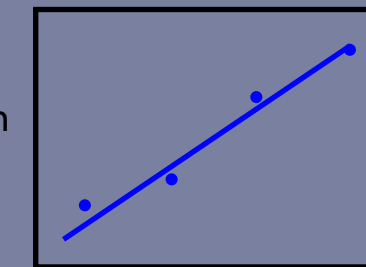
Local environment variation induced by adsorbates

Analytic linear relationships

0.25 ML 0.50 ML 0.75 ML 1.00 ML
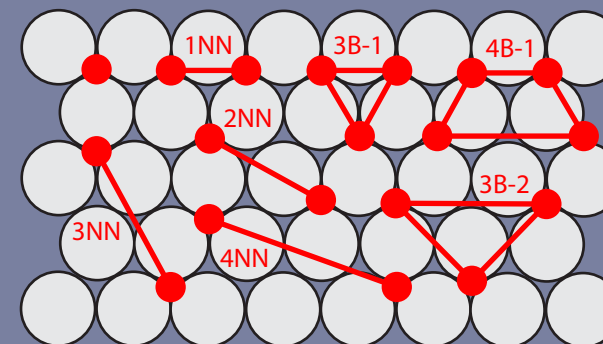
Adsorption Energy

Coverage

ML-parameterized cluster expansions

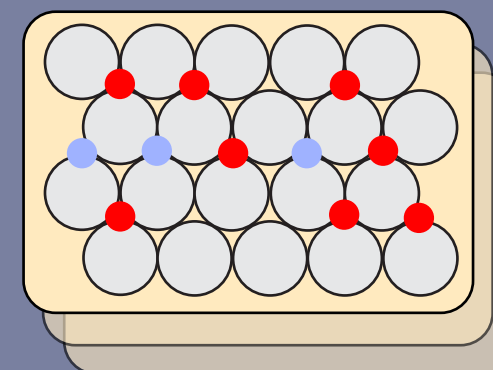1NN 3B-1 4B-1
2NN
3NN 3B-2
4NN

Cross Validation

Parameterization

Regularization

Pattern Recognition

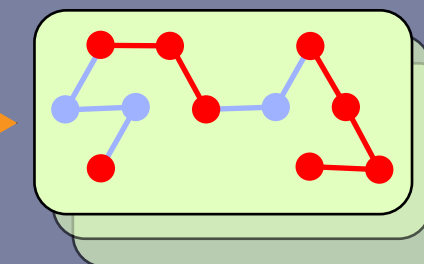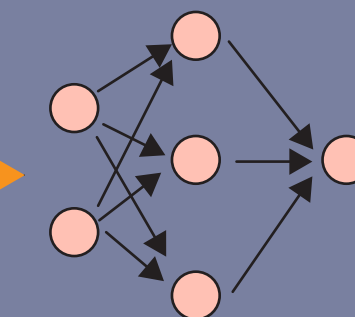**Highly nonlinear deep learning models**

Surface configurations

Surface graph representation

Convolutional layers

Hidden layers

Output