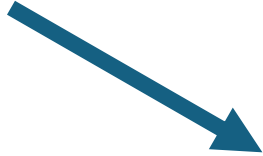


1. understand the problem

adsorption energy as a measure how strongly a molecule binds to a surface



2. collect the data

*DFT databases
catalysis-hub.org
OC20 / OC22
Materials Project
NOMAD repository

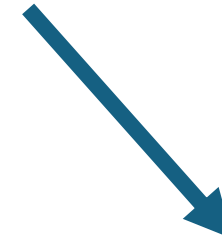
*VASP, Quantum ESPRESSO, or ASE



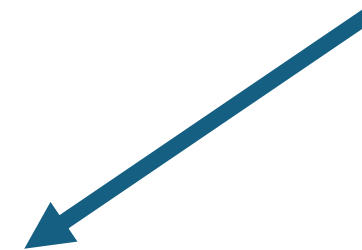
3. feature engineering

*surface descriptors
*adsorbate descriptors

Molecular fingerprints (Morgan, MACCS), Surface Miller index, Structure-based features.



4. feed the ML models + evaluate the results



5. write the thesis!!!