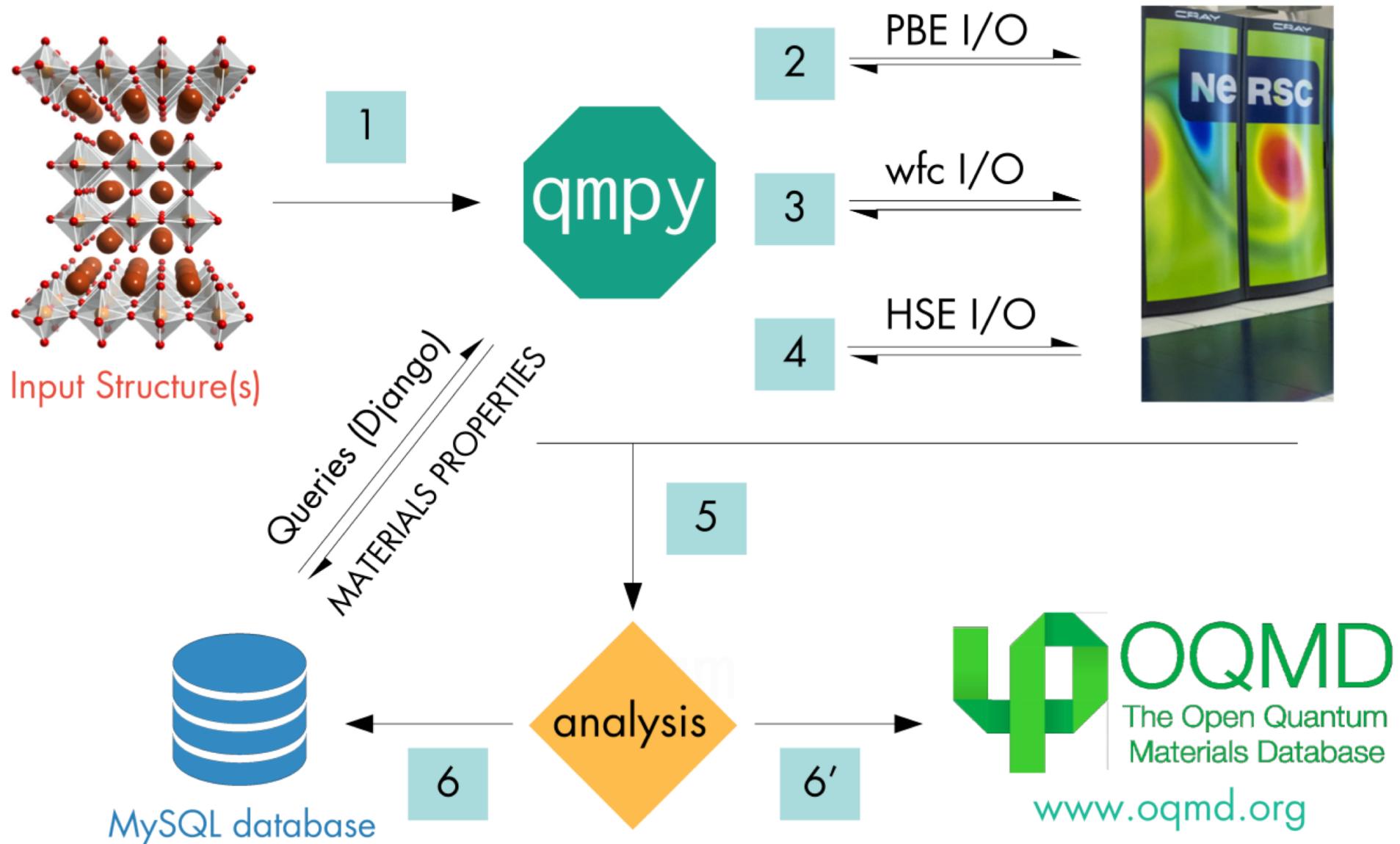
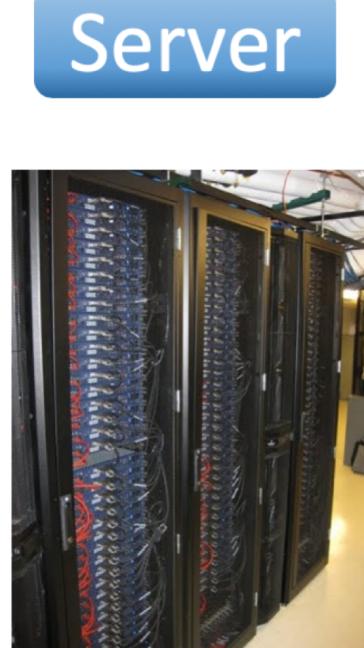


# Workflow of OQMD



# Workflow of OQMD API



OQMD (MySQL)



↔  
*qmpy (django)*



GET data through  
HTTP request

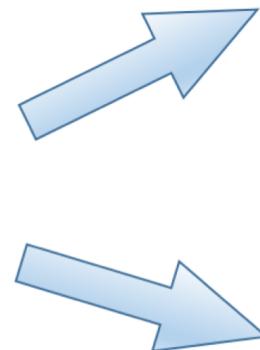
Client

**OQMD:**  
*An Open Quantum Materials Database*

<http://oqmd.org>

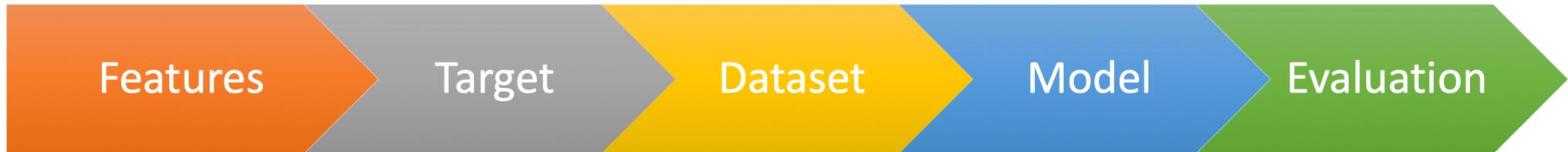


*QMPYRest()*



Web Search Interface

# Workflow of ML on Materials



Generalized  
elemental properties  
(Magpie)

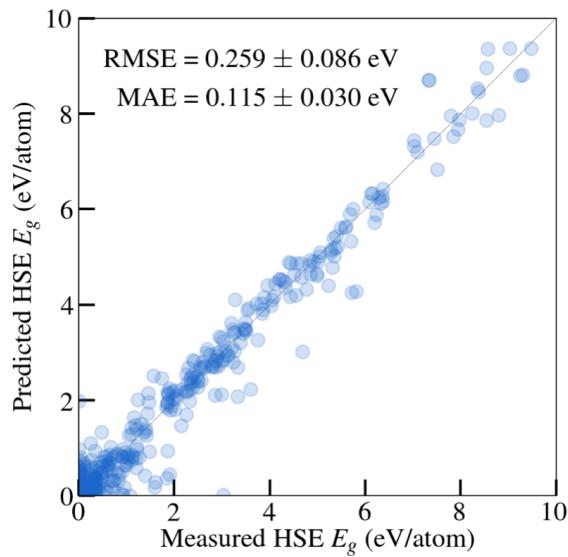
Experiment data  
& High-fidelity  
computational data

Materials properties  
data stored in  
OQMD (low-fidelity)

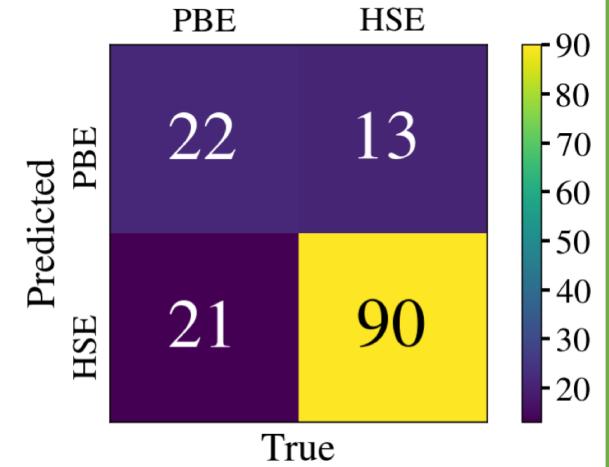
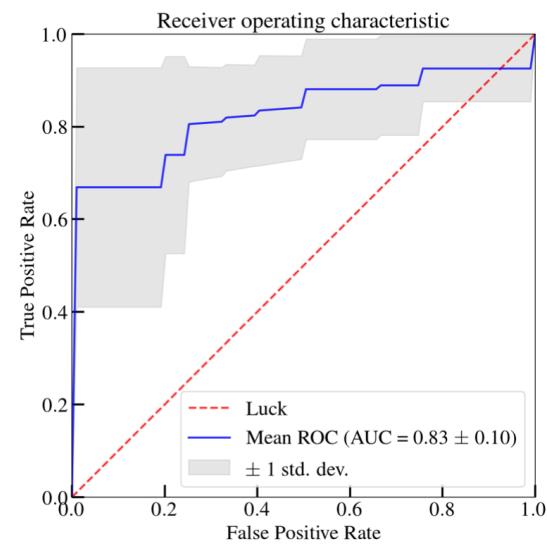
LASSO  
SVM  
Random Forest

10-fold cross-validation  
Both RMSE & MAE

## Regression Model on high-fidelity data prediction



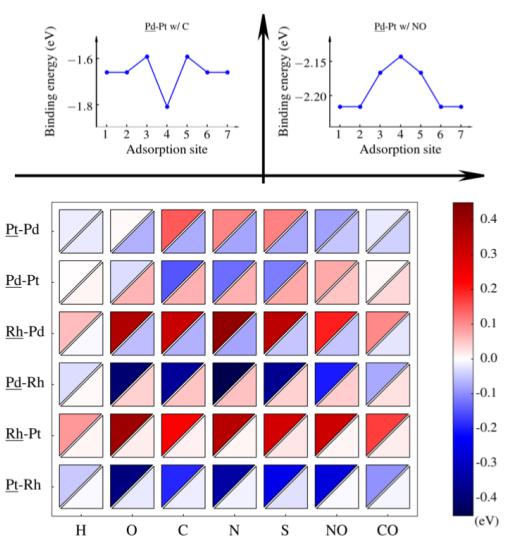
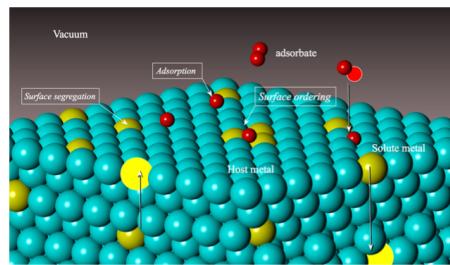
## Classification Model on whether high-fidelity calculation is needed



# Catalyst design and discovery

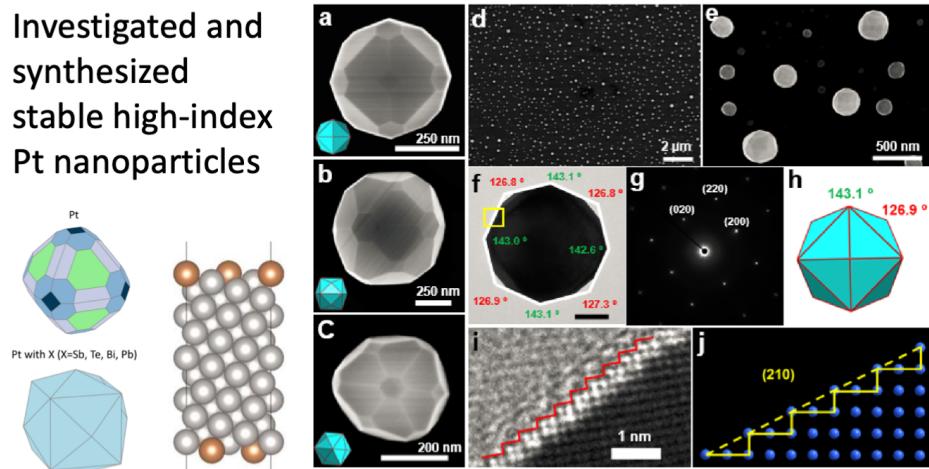
## Fundamental Study

Provided insight into the interplay of compositional and atomic ordering on adsorption at surface alloys



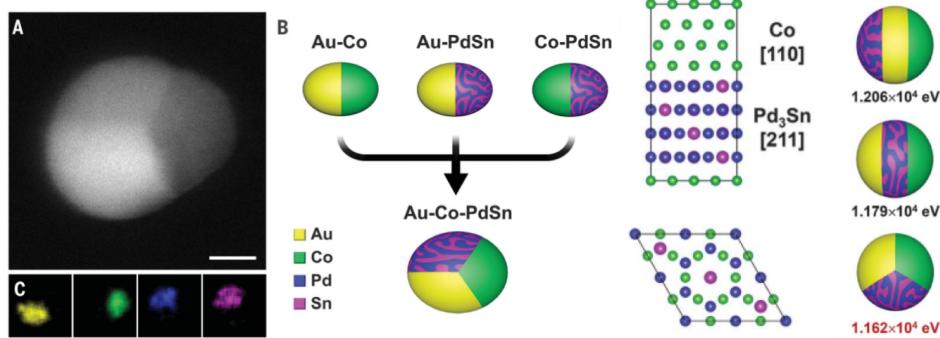
## Surface Stability

Investigated and synthesized stable high-index Pt nanoparticles



## Interface Design

Established design rules for making poly-elemental nanoparticles with specific interfaces and heterostructures.



## Catalytical Activities

Designed and discovered Pt-Au-Cu ternary nanoparticles: optimal hydrogen evolution reaction catalyst

