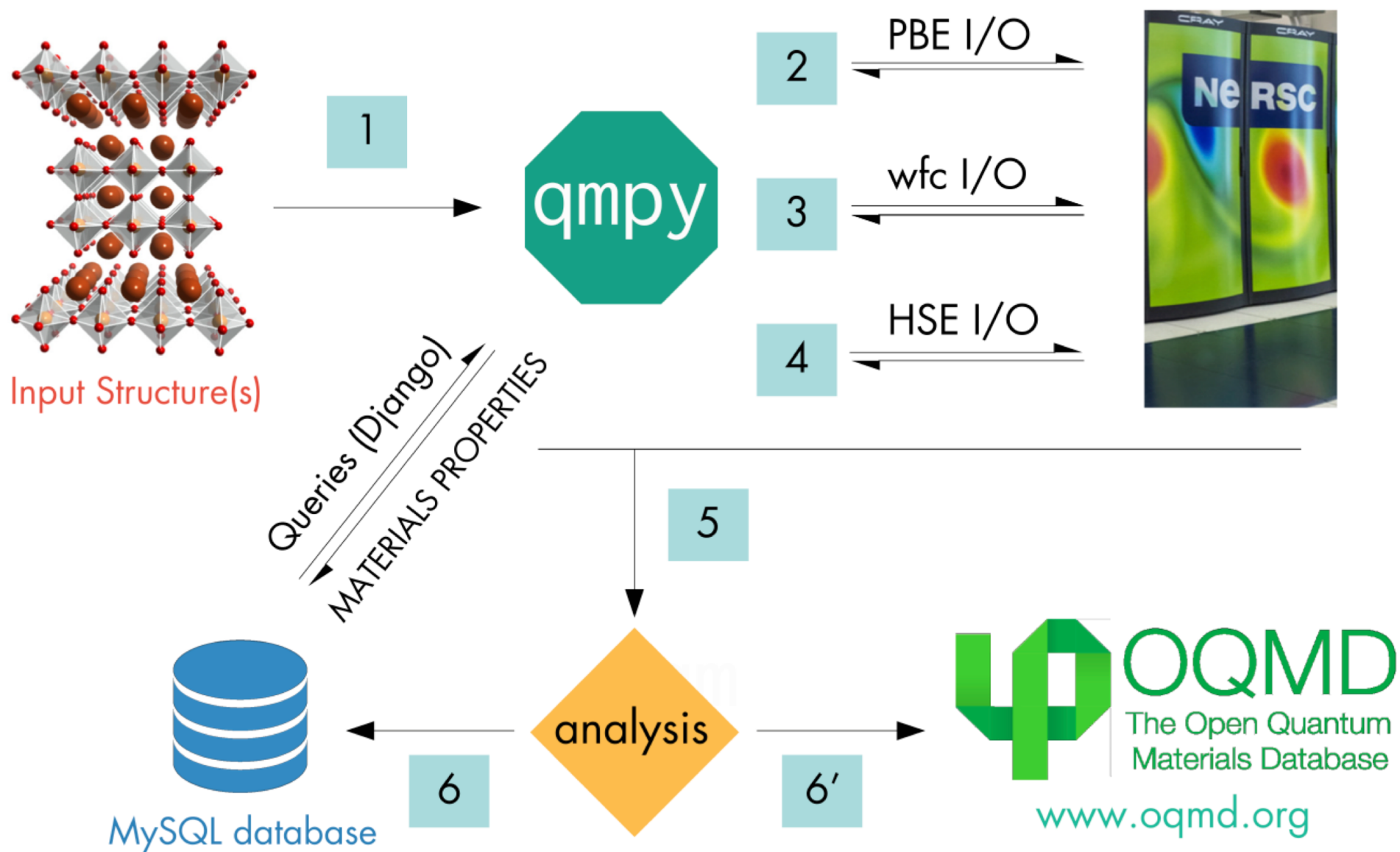


Workflow of OQMD



Workflow of OQMDAPI

Server



OQMD (MySQL)



qmpy (django)

OQMDAPI



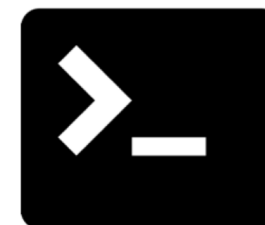
GET data through
HTTP request

Client

OQMD:

An Open Quantum Materials Database

<http://oqmd.org>

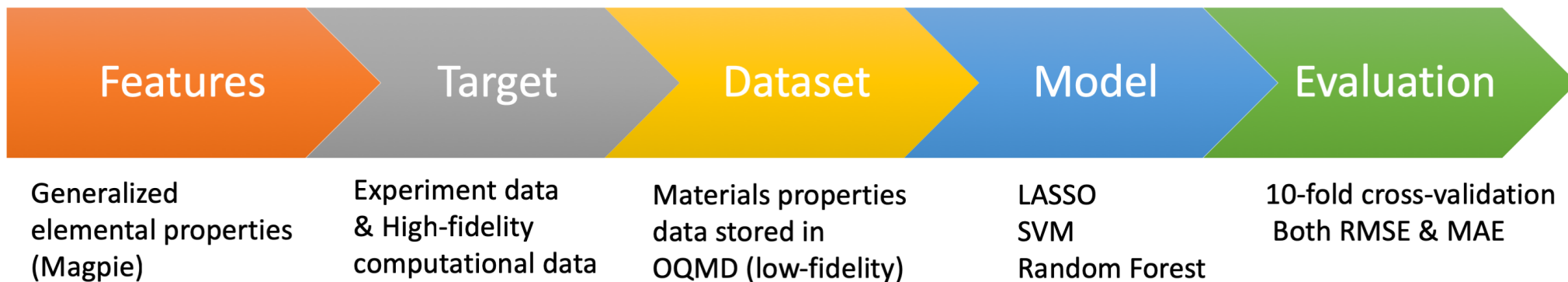


QMPYRester()

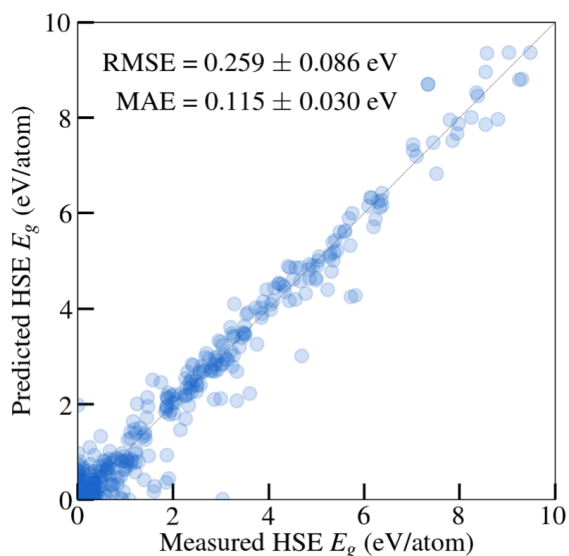


Web Search Interface

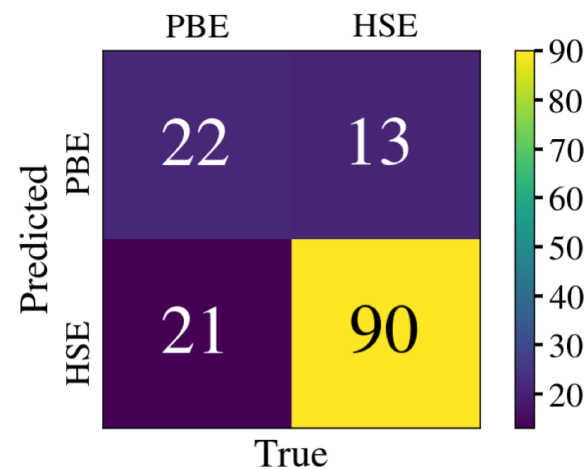
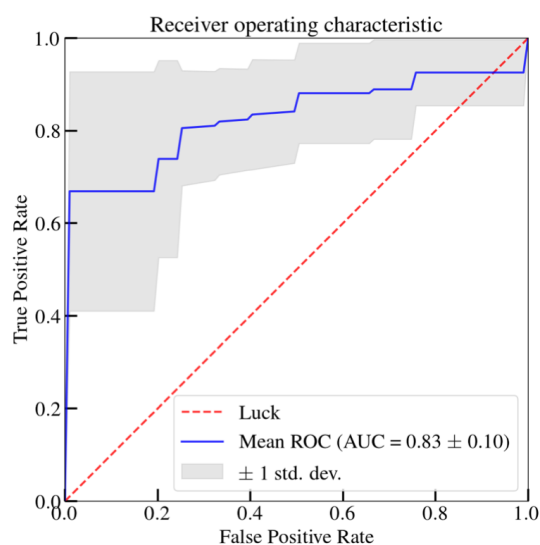
Workflow of ML on Materials



Regression Model on high-fidelity data prediction



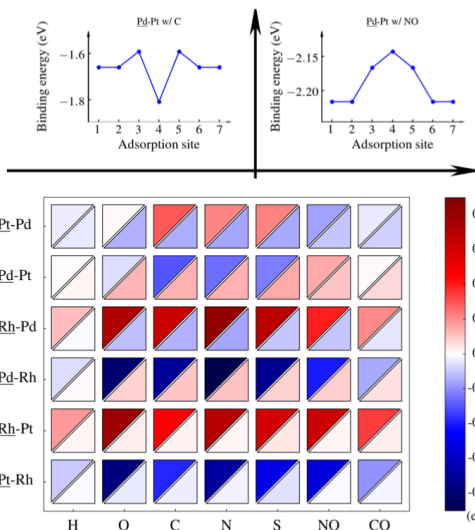
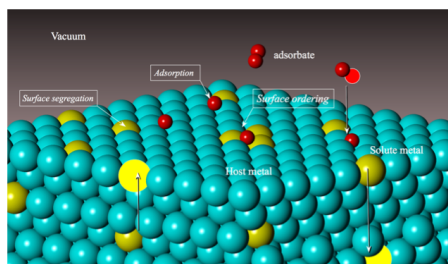
Classification Model on whether high-fidelity calculation is needed



Catalyst design and discovery

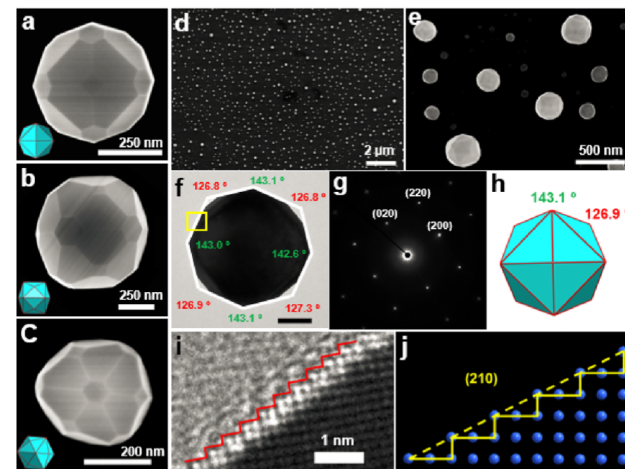
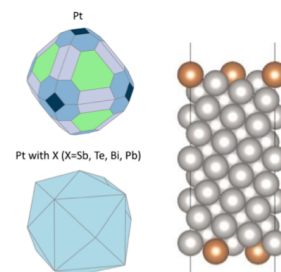
Fundamental Study

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



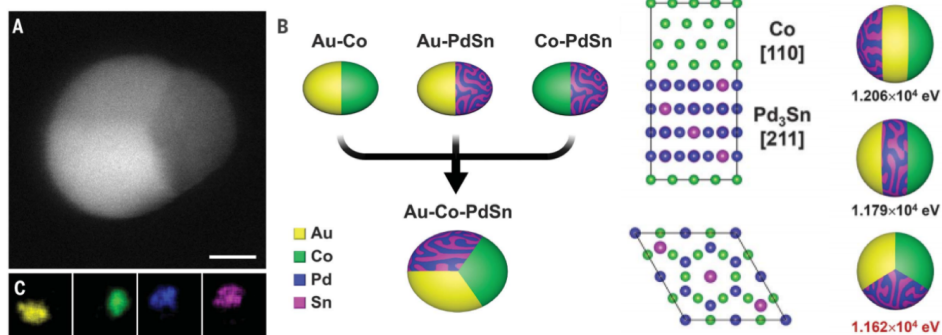
Surface Stability

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

