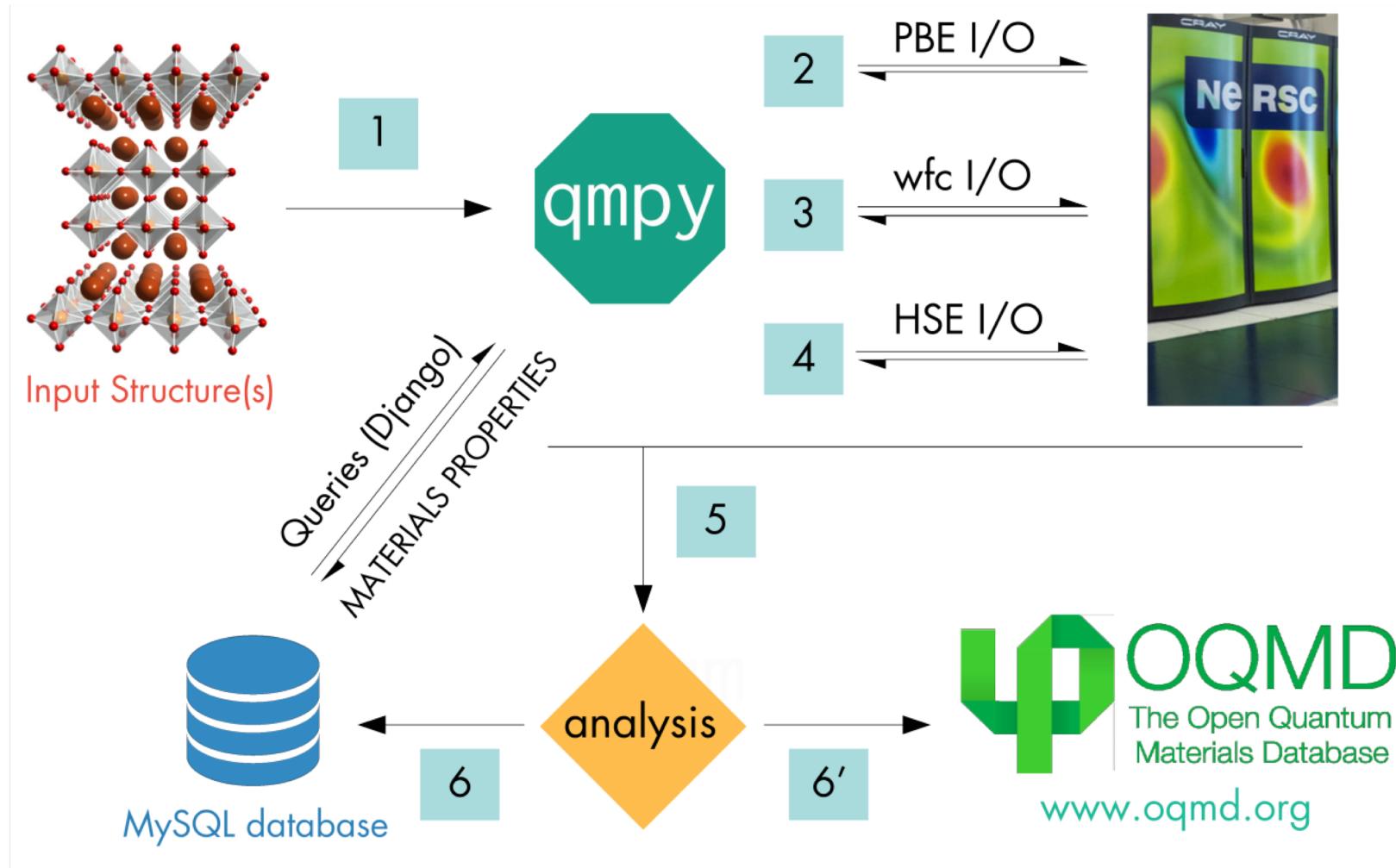


Workflow of OQMD



Workflow of OQMD API

Server



OQMD (MySQL)



qmpy (django)

OQMD API

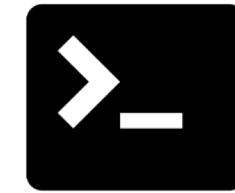


GET data through
HTTP request

Client

OQMD:
An Open Quantum Materials Database

<http://oqmd.org>

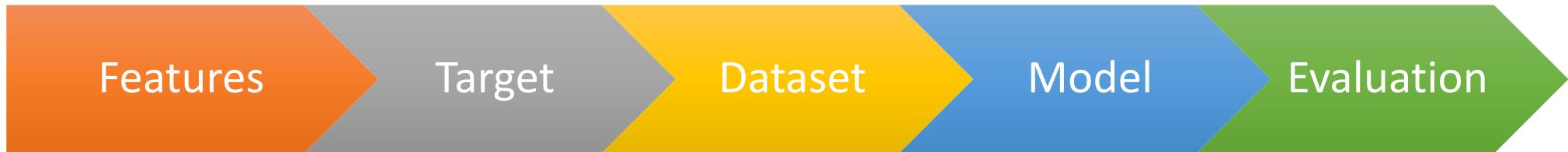


QMPYRester()



Web Search Interface

Workflow of ML on Materials



Generalized
elemental properties
(Magpie)

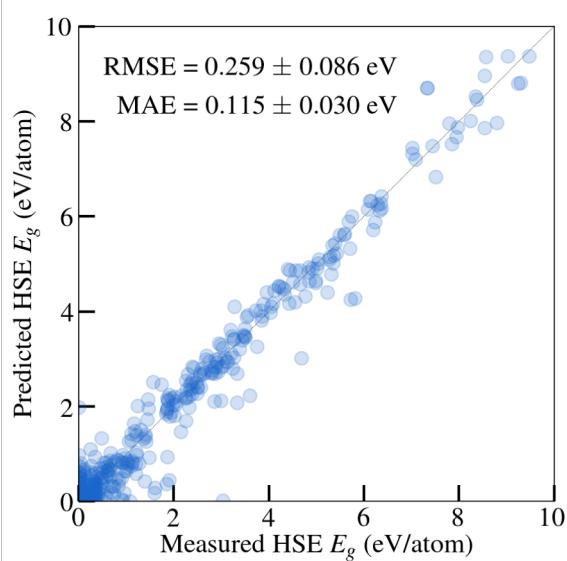
Experiment data
& High-fidelity
computational data

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

