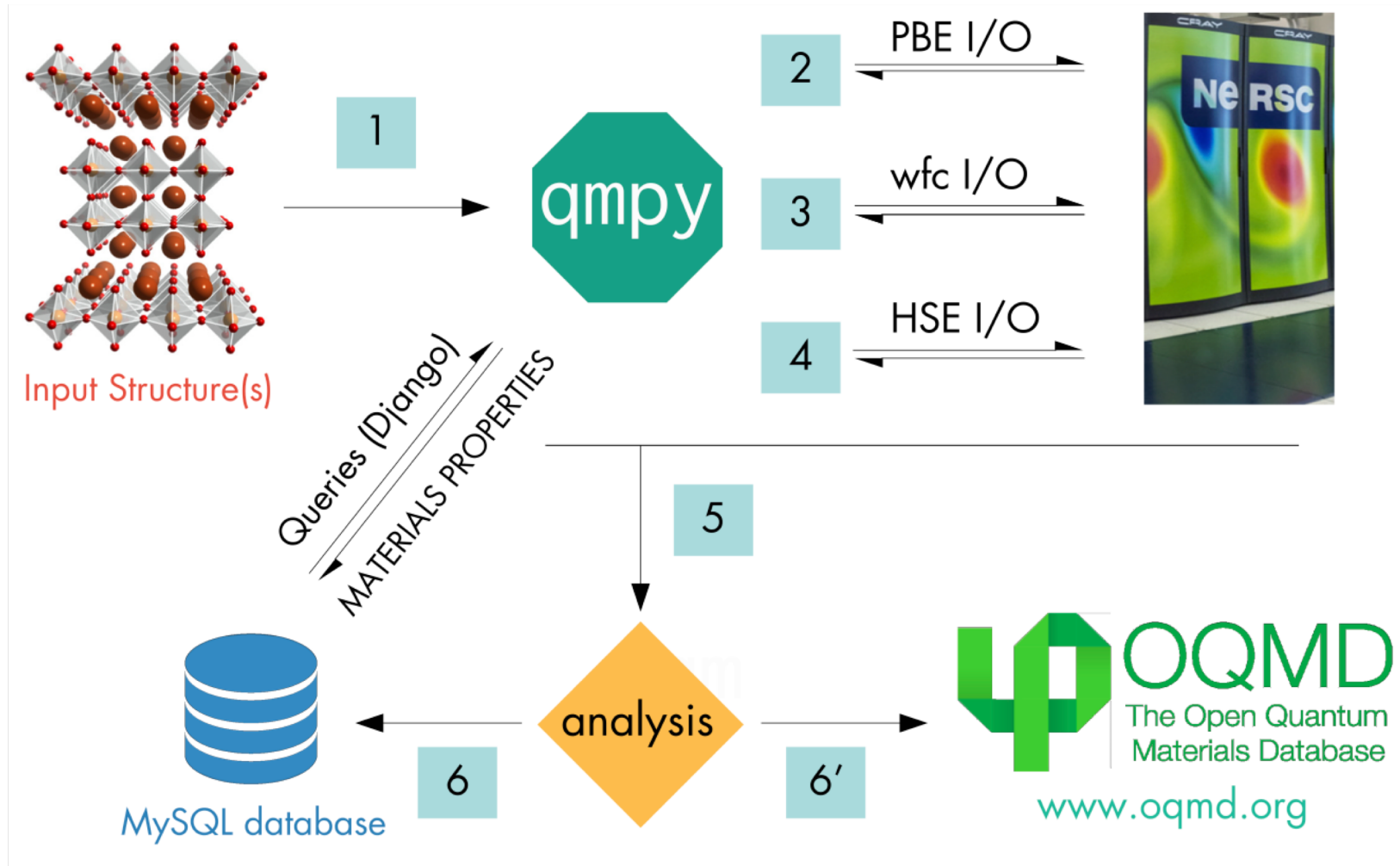


Workflow of OQMD



Workflow of OQMDAPI

Server



OQMD (MySQL)



qmpy (django)

OQMDAPI



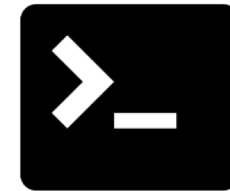
GET data through
HTTP request

Client

OQMD:

An Open Quantum Materials Database

<http://oqmd.org>



QMPYRest()



Web Search Interface



Magpie Features
PBE bandgaps

Experimental
bandgaps

Exp from two sources
PBE from MP

KRR
LASSO

LOOCV-RMSE using
KRR = 0.51 eV (Magpie)
LASSO = 0.71 eV (Magpie)
KRR = 0.34 (w/ MP_PBE)

