

Start gmx2qmmm.py

userInputs

gmx2qmmm

Instantiation of QMMMInputs class

perform\_job

perform\_opt

get\_energy

Subprocess gmx & g16

while not done:

opt\_cycle

maxforce < force threshold?

yes

done

no

make\_opt\_step

make\_new\_g96

qmmm\_prep

readg96

readmols

readcharges

\_helper.py

make\_xyzq

prepare\_pcf\_for\_shift\_fieldonly

get\_linkatoms\_ang

generate\_charge\_shift\_fieldonly

get\_energy

Subprocess gmx & g16

ending criterion met?

yes

done

no

gmx2qmmm.py

readInput.py

qmmm.py

generate\_pcf\_from\_top.py

prepare\_pcf\_for\_shift.py

generate\_charge\_shift.py