gmx2qmmm.py

Start gmx2qmmm.py

userInputs

gmx2qmmm

readInput.py

Instantiation of QMMMInputs class

perform_job

qmmm.py

perform_opt

get_energy

Subprocess gmx & g16

while not done:

opt_cycle

maxforce < force threshold?

yes

no

done

make_opt_step

make_new_g96

qmmm_prep

generate_pcf_from_top.py

readg96

readmols

readcharges

_helper.py

make_xyzq

prepare_pcf_for_shift.py

prepare_pcf_for_shift_fieldsonly

get_linkatoms_ang

generate_charge_shift.py

generate_charge_shift_fieldsonly

get_energy

Subprocess gmx & g16

ending criterion met?

yes

no

done

Instantiation of QMMMInputs

Instatiation of MMParams

→ Reads information from mm.dat

Instatiation of QMParams

→ Reads information from qm.dat

Instatiation of PathParams

→ Reads information from path.dat

Instatiation of QMMMParams

→ Reads information from qmmm.dat

Read molecules from topology

Read charges of all atoms in all molecules

Read xyz for all atoms

Read number of atoms from structure file

Read connection of atoms from topology

Read qm atoms

If inout: make inner/outer list

If structure file is gro: write to g96

Make xyzq

Get m1 and m2 atoms and shift charges

Get vector from qm atom to mm atom if bond is cut

Get_linkcorrlist?

Class MMParams

read_mmparams

Class QMParams

read_qmparams

Class PathParams

read_pathparams

Class QMMMParams

read_qmmmparams

readmols

readcharges

checkformol

readg96

read_numatoms

read_conn_list_from_top

get_curr_top

checkformol

get_mollength_direct

get_connlist

read_qmatom_list

read_inner_list

read_outer_list

write_highprec

stepper

make_xyzq

prepare_pfc_for_shit_fieldsonly

identify_m1

get_bondpartners

identify_m2

get_bondpartners

get_qmcoords

eliminate_and_shift_to_m1

get_linkatoms_ang

get_linkcorrlist

readInput.py

generate_pcf_from_top.py

prepare_pcf_for_shift.py

_helper.py

generate_charge_shift.py

sum_pcf_tm.py

generate_top.py

Make new point charge field

Calculate distance vectors * charge for m/q atoms

While loop until maximum displacement below threshold

Write new topology