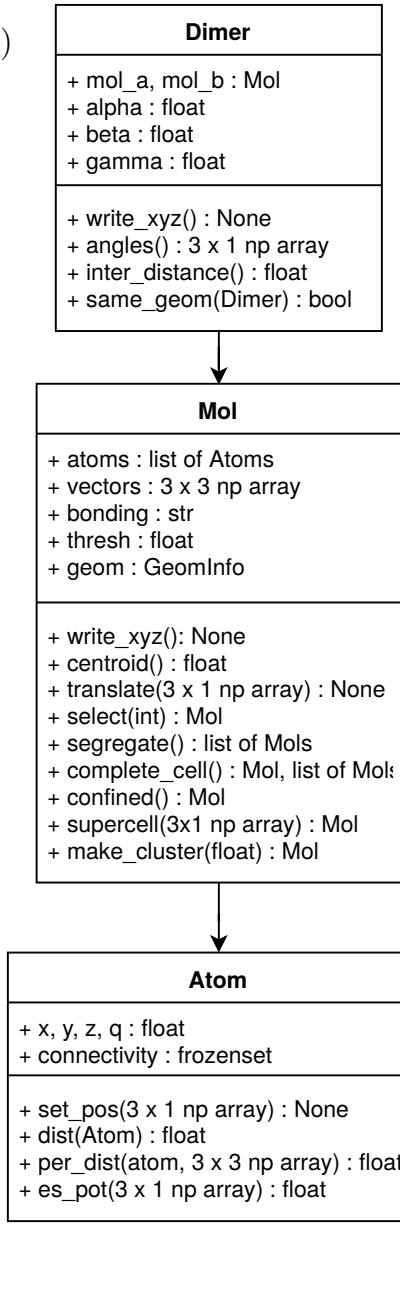
a)



b)

- **fro_assign_charges.py**

  Redistribute partial atomic charges onto an aggregate via connectivity

- **fro_coupling.py**

  Evaluate the exciton coupling in a given dimer

- **fro_exciton classification.py**

  Calculate indices classifying a TDDFT excited state as a localised, delocalised, or CT exciton

- **fro_dimer_tools.py**

  Extract the unique dimers from a unit cell or aggregate and analyse their conformations

- **fro_uc_tools.py**

  Use a unit cell to produce a supercell, molecular cluster or other aggregate geometry

- **fro_volumetrics.py**

  Analyse the available volume of a fragment in an aggregate geometry and print it out as a cube file

- **fro_prep_run.py**

  Starting from a unit cell geometry, produce the necessary template files and embedding charges for an ONIOM cluster model calculation

- **fro_run.py**

  Perform a geometry optimisation to find an energy minimum or MECI using an ONIOM cluster model across a range of electronic structure programs