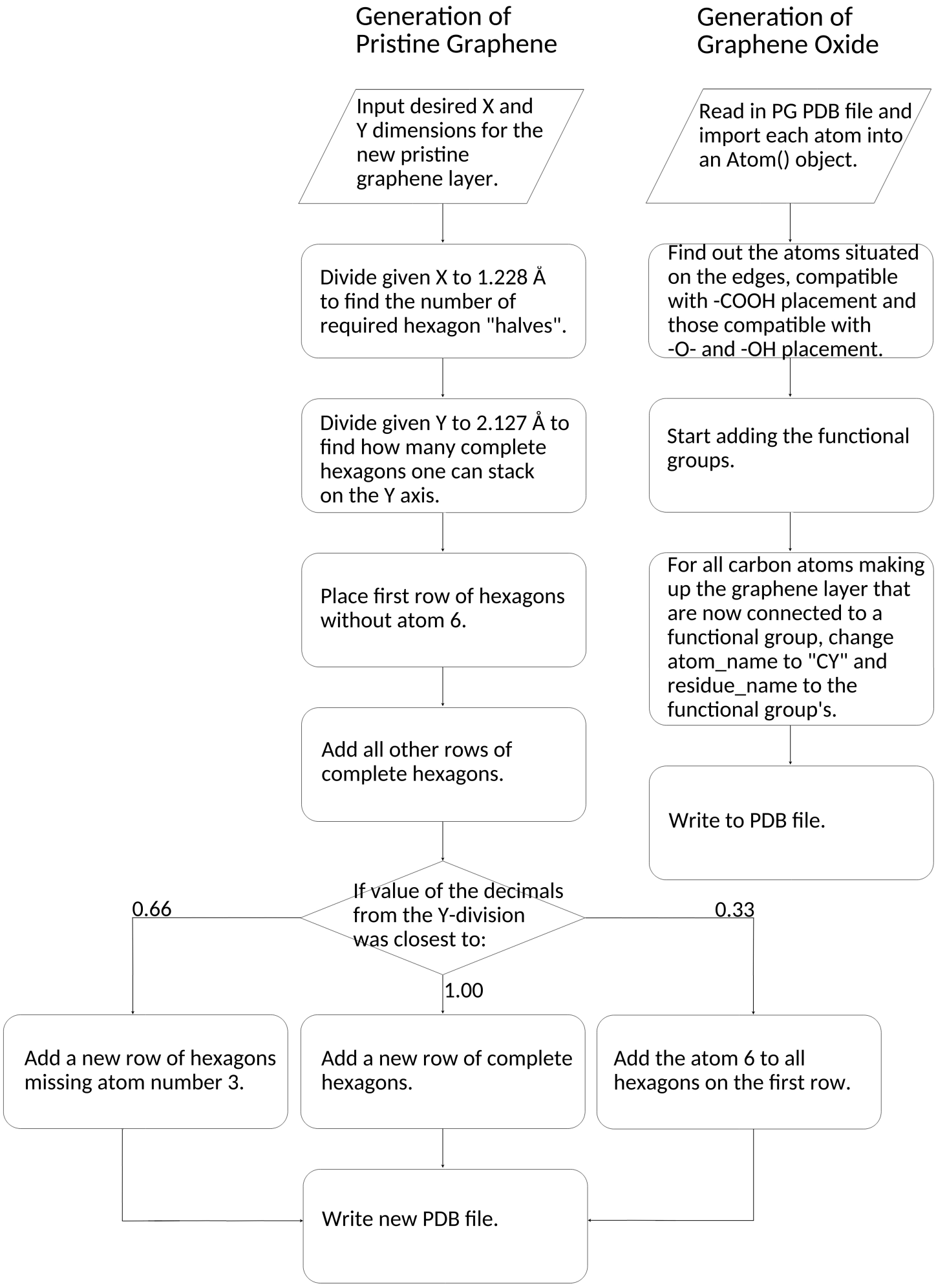
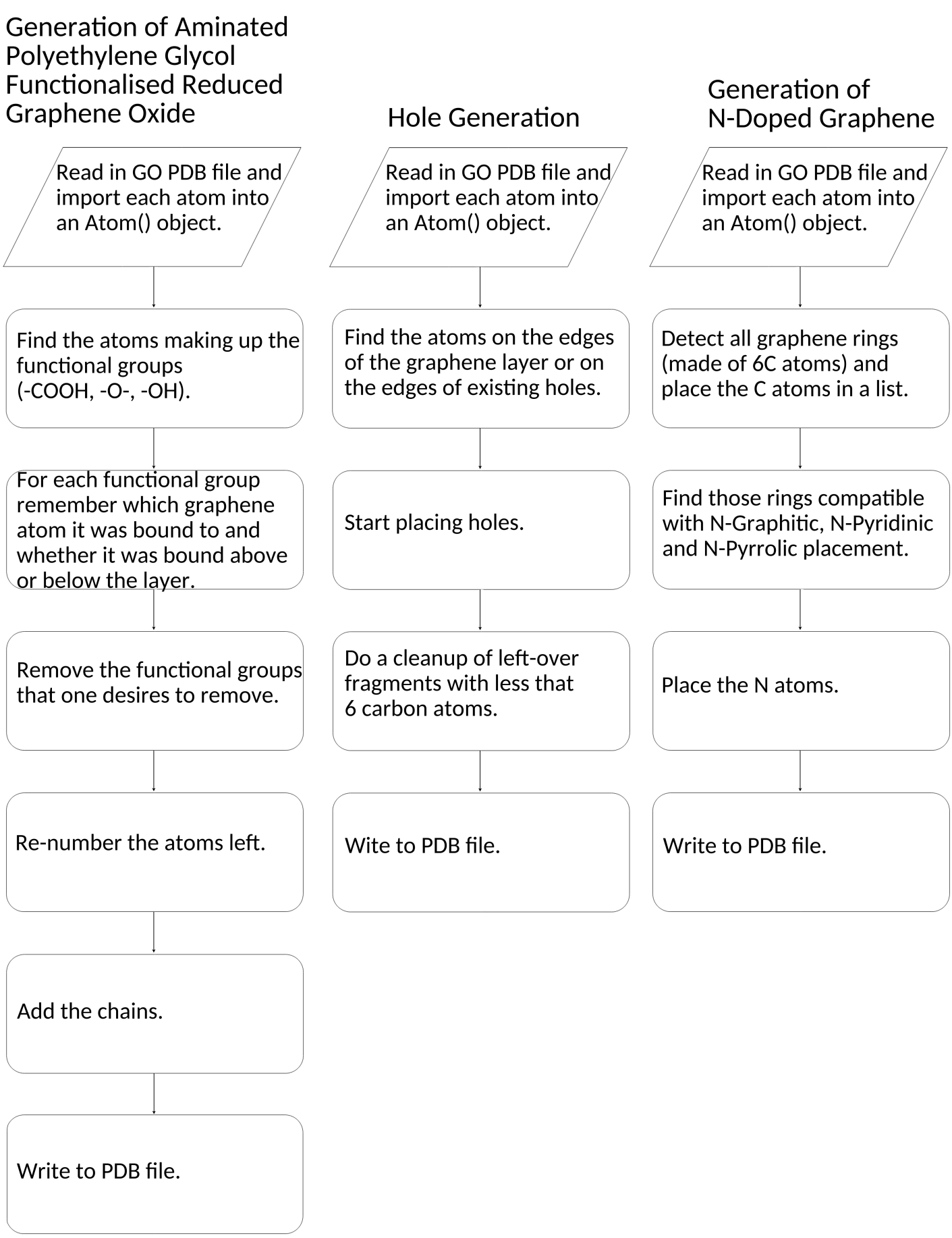

Generation of Pristine Graphene
Input desired X and Y dimensions for the new pristine graphene layer.
Divide given X to 1.228 Å to find the number of required hexagon "halves".
Divide given Y to 2.127 Å to find how many complete hexagons one can stack on the Y axis.
Place first row of hexagons without atom 6.
Add all other rows of complete hexagons.
If value of the decimals from the Y-division was closest to:
0.66
1.00
0.33
Add a new row of hexagons missing atom number 3.
Add a new row of complete hexagons.
Add the atom 6 to all hexagons on the first row.
Write new PDB file.
Generation of Graphene Oxide
Read in PG PDB file and import each atom into an Atom() object.
Find out the atoms situated on the edges, compatible with -COOH placement and those compatible with -O- and -OH placement.
Start adding the functional groups.
For all carbon atoms making up the graphene layer that are now connected to a functional group, change atom_name to "CY" and residue_name to the functional group's.
Write to PDB file.



Supplementary Figure 2. Flow charts summarizing the steps taken for each of the five functionalities of GOPY.