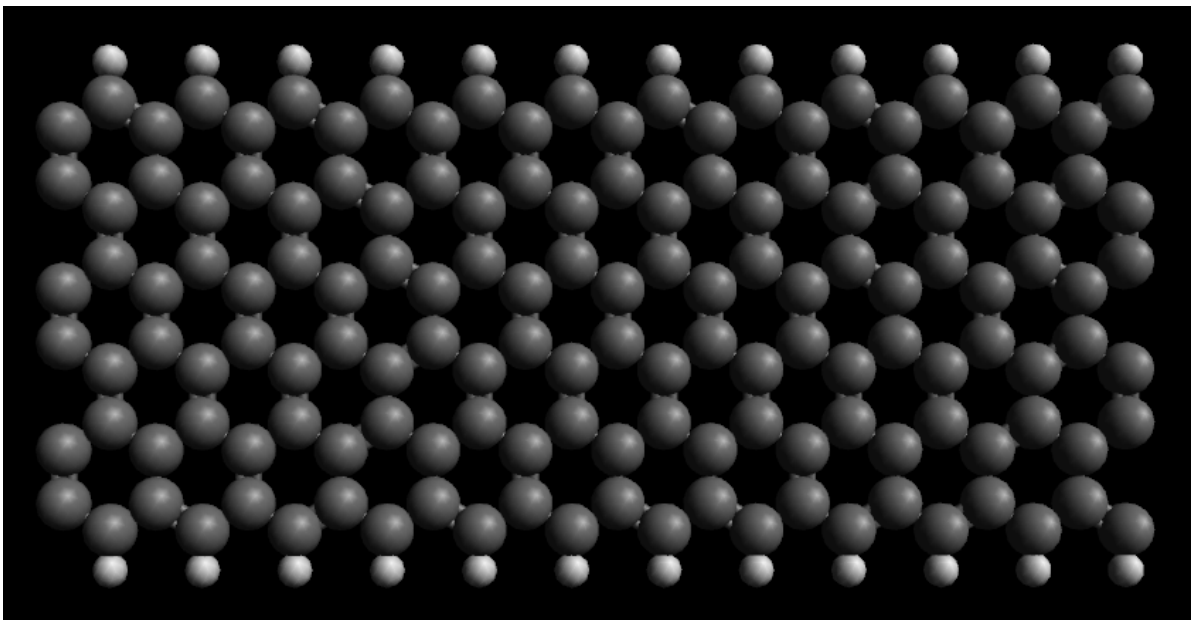
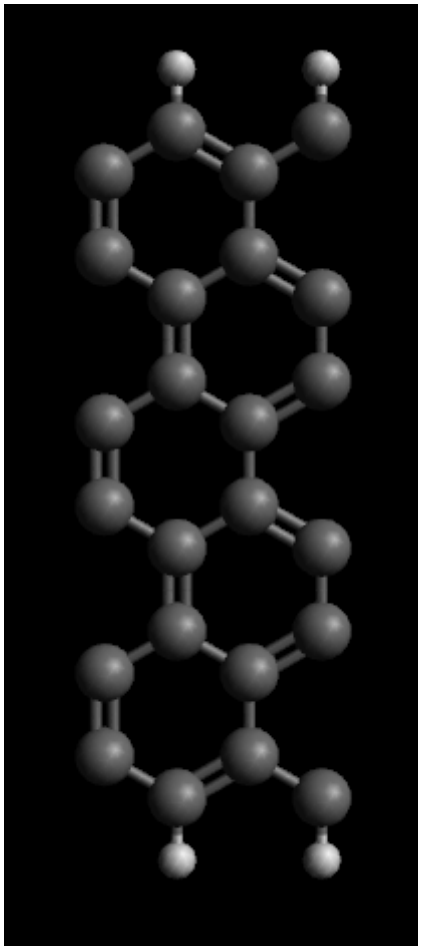
Doping Graphene Nano Ribbon(GNR) with Nitrogen and Bohr in order to reach semiconductor behavior

basic description

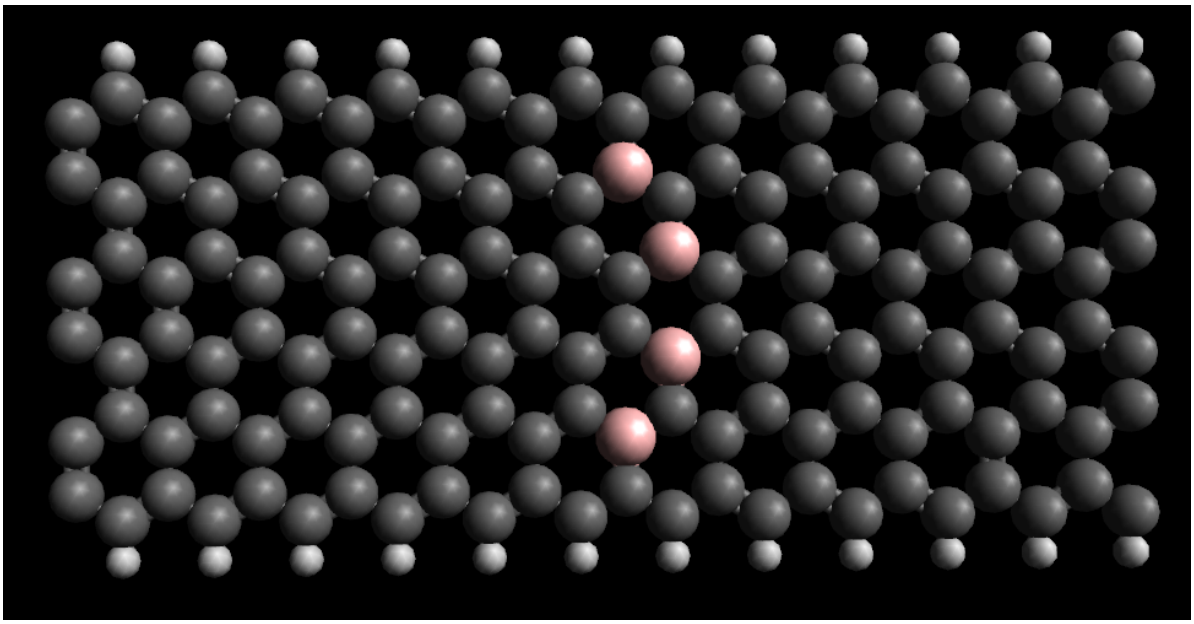
In this project, the basic structure of zzGNR (with 12 layers, 12 Carbon and 2 Hydrogen atoms each -> total 168 atoms) is considered



And the side 2 layers are used as electrodes



Electron transport and DOS for the pure zzGNR and the doped one is simulated using SIESTA/TRanSIESTA software. The doping positions is shown in the picture below



Software material

- SIESTA Package version 4.0 is used for the simulations.
- Avogadro Software is used to visualize the atomic structure
- GnuPlot is used to plot the results

Method

GGA/PBE method is used

Geometric notes

C-C bond length of 1.433600 Ang is used and C-H bond length of 0.75*1.433600 Ang

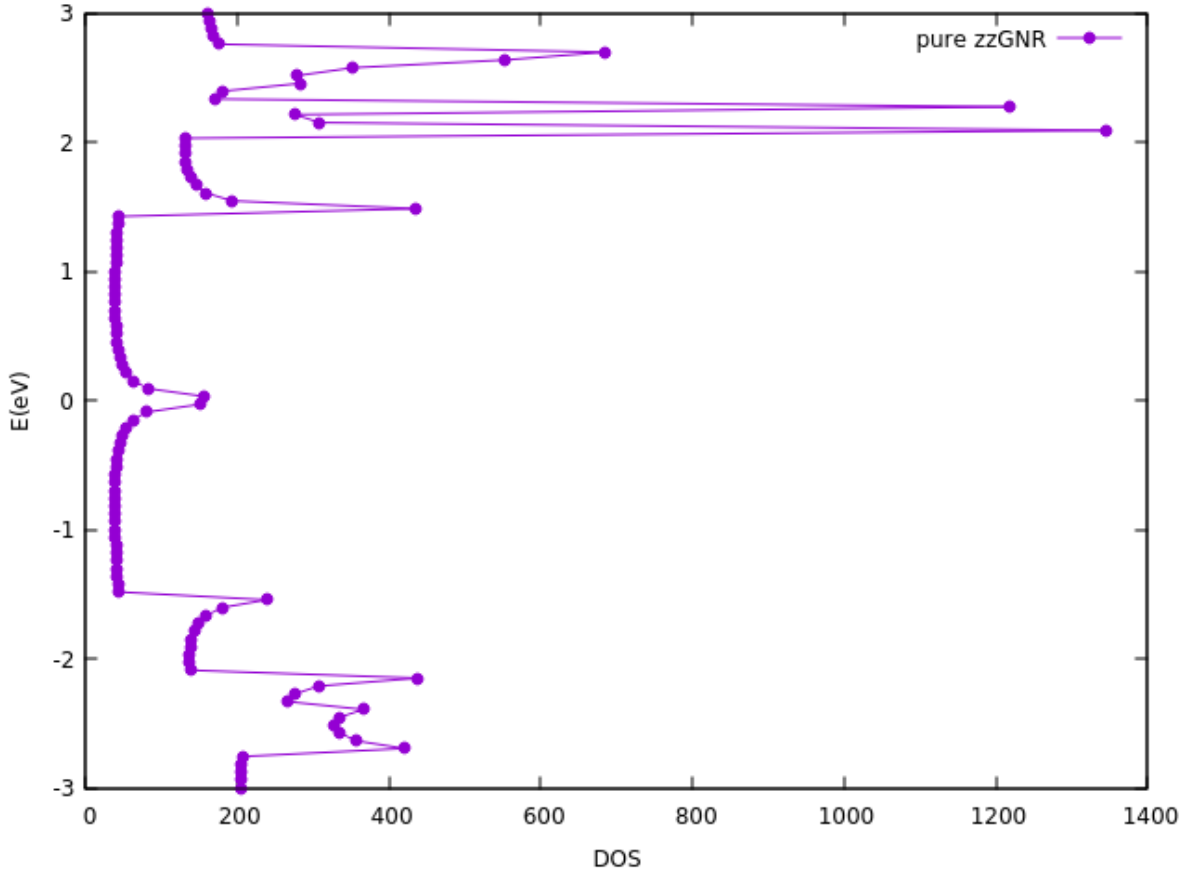
After some unsuccessful tries to Relax the structure (divergence of SCF algorithm) , duo to unfamiliarity with Geometric optimization algorithms, we gave up this part

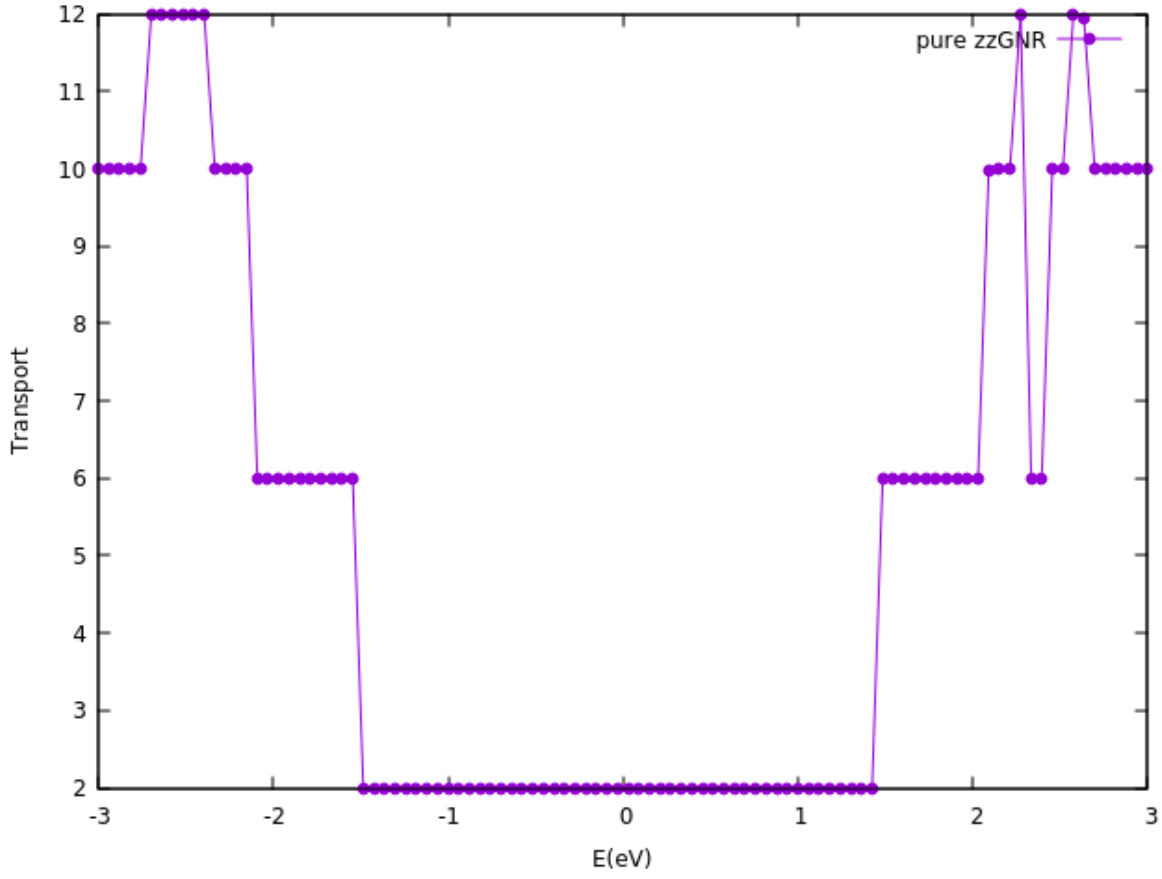
Results

The DOS and electron transport for the pure zzGNR

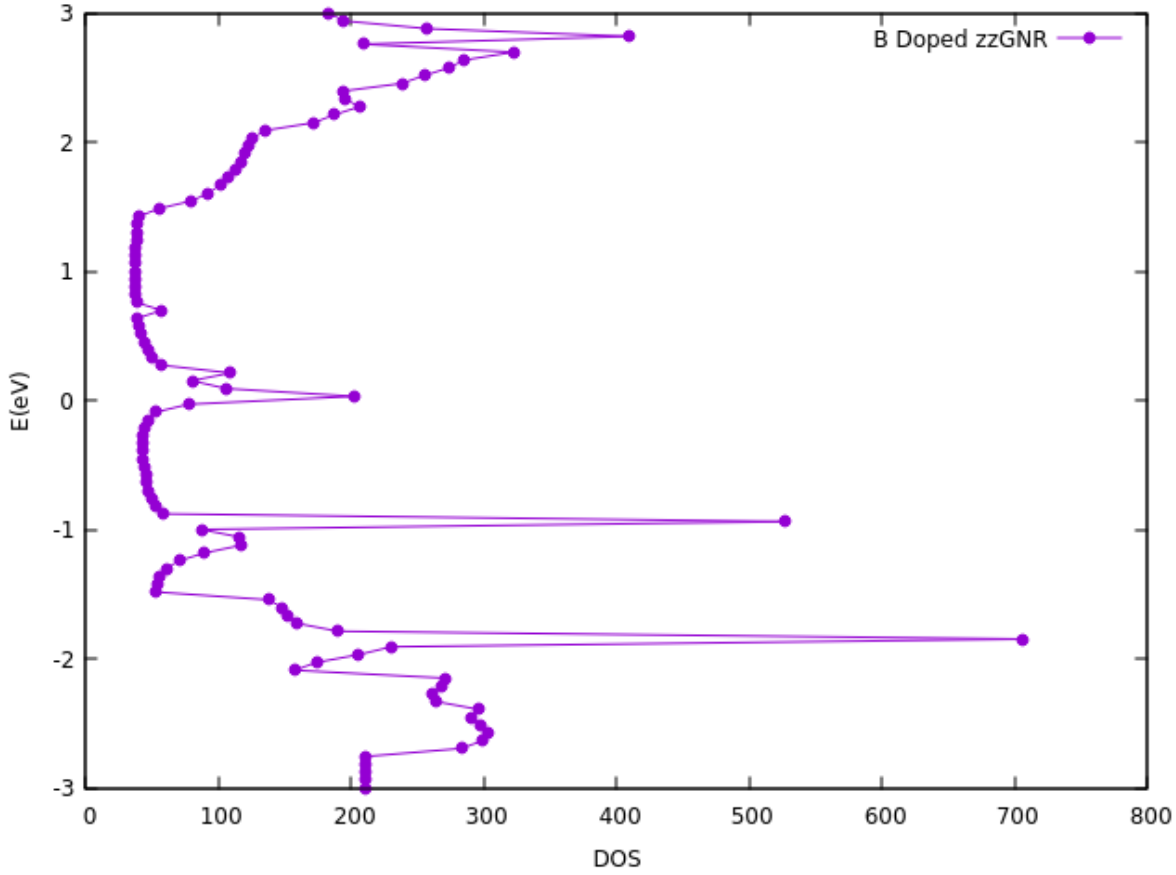
note that in the results, E is actually: E-E_f

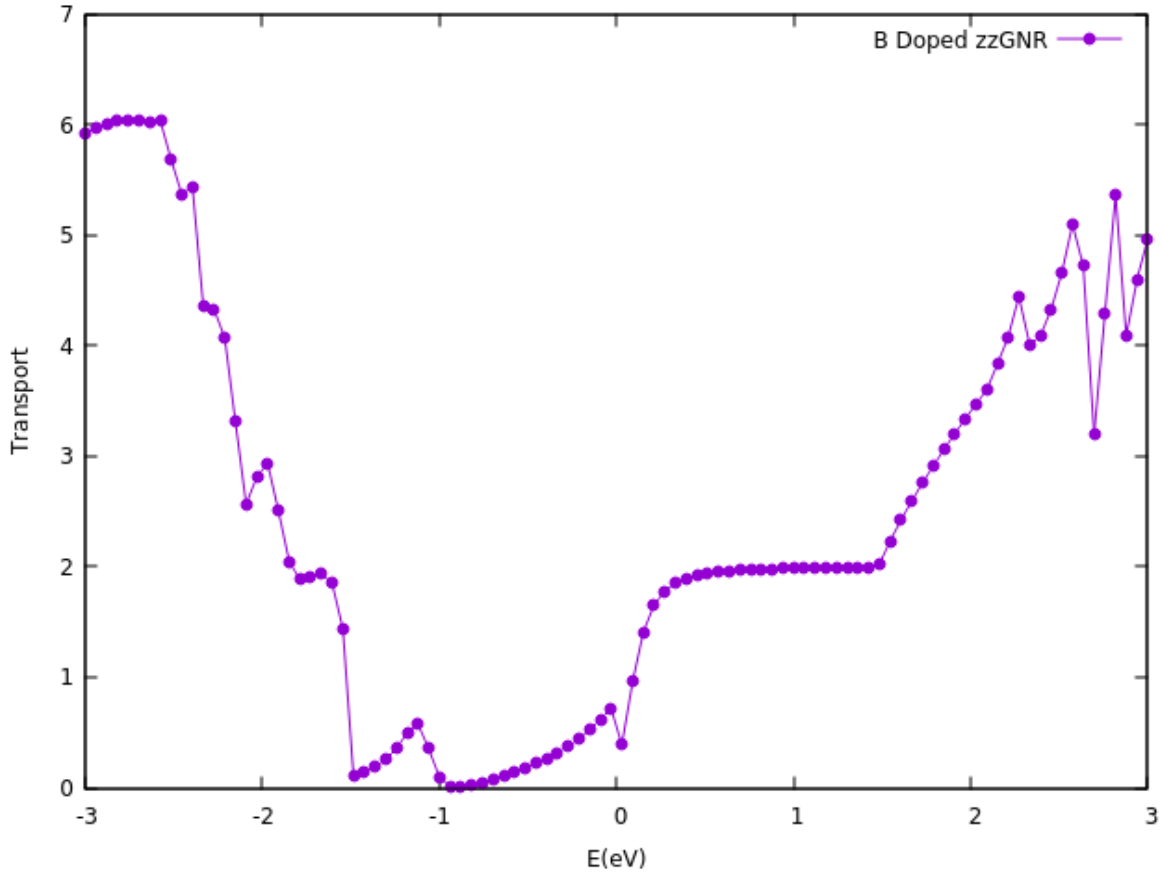
and Bias (V) = 0



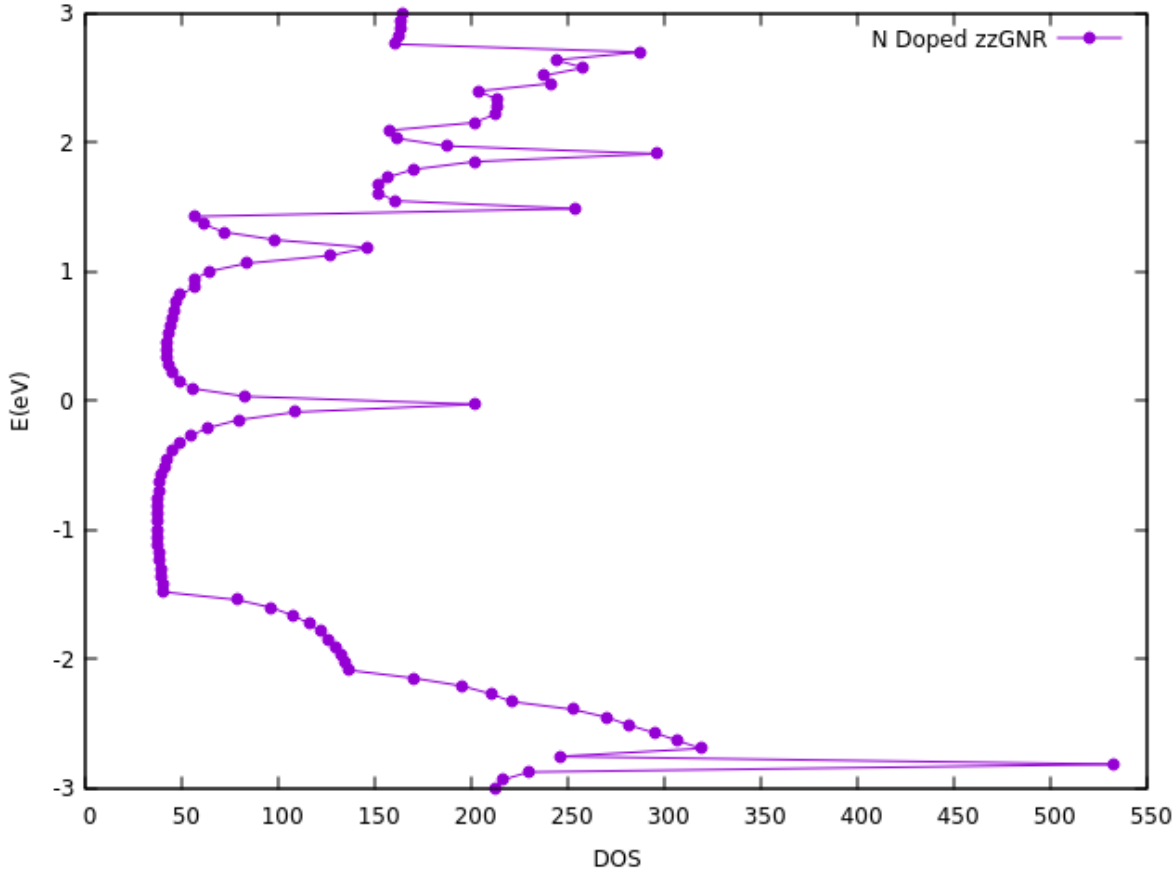


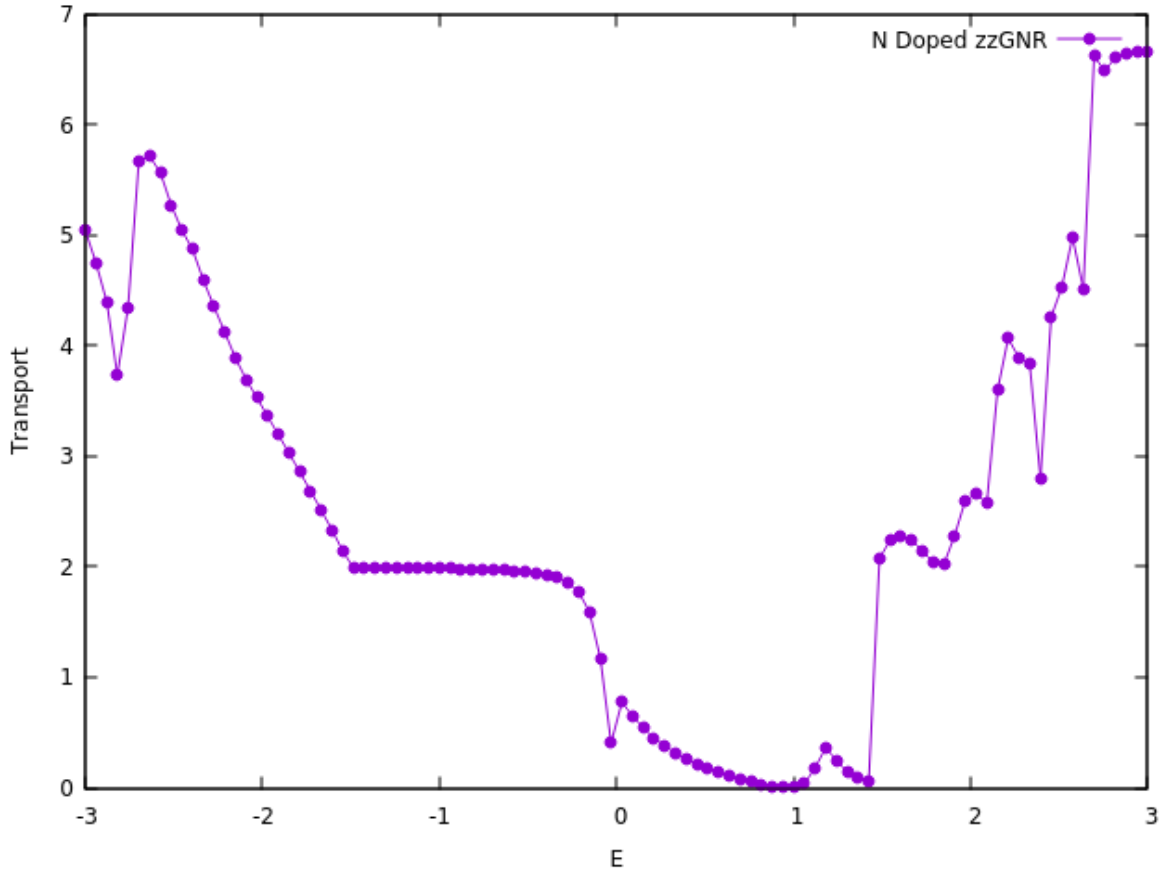
After doping with 4 Bohr atoms in certain positions, as it's visible in the DOS, some states are appeared below the fermi level; so the B doped zzGNR can show behavior of a p-type semiconductor





And so for the N doped case, the density of states, is stronger ahead of the fermi level.


N Doped zzGNR
E(eV)
DOS
3
2
1
0
-1
-2
-3
0
50
100
150
200
250
300
350
400
450
500
550


N Doped zzGNR
Transport
E
7
6
5
4
3
2
1
0
-3
-2
-1
0
1
2
3