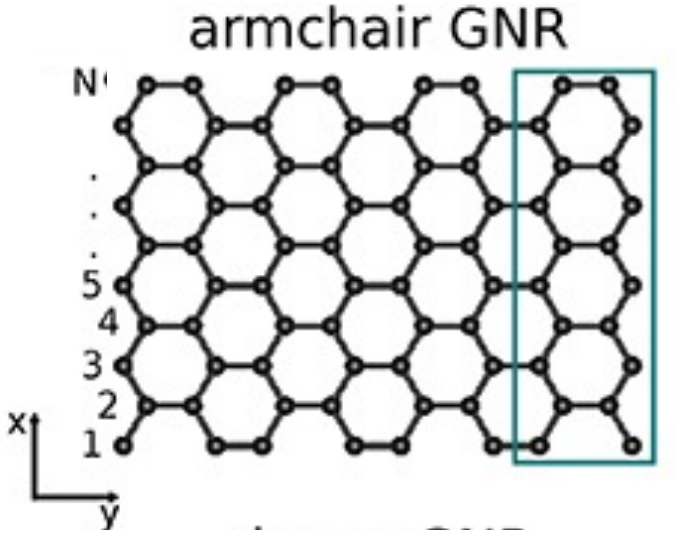
Exercise 2: graphene nanoribbon (1D system)

Go to: **/scratch/esc#/EXERCISE_3_GNR**

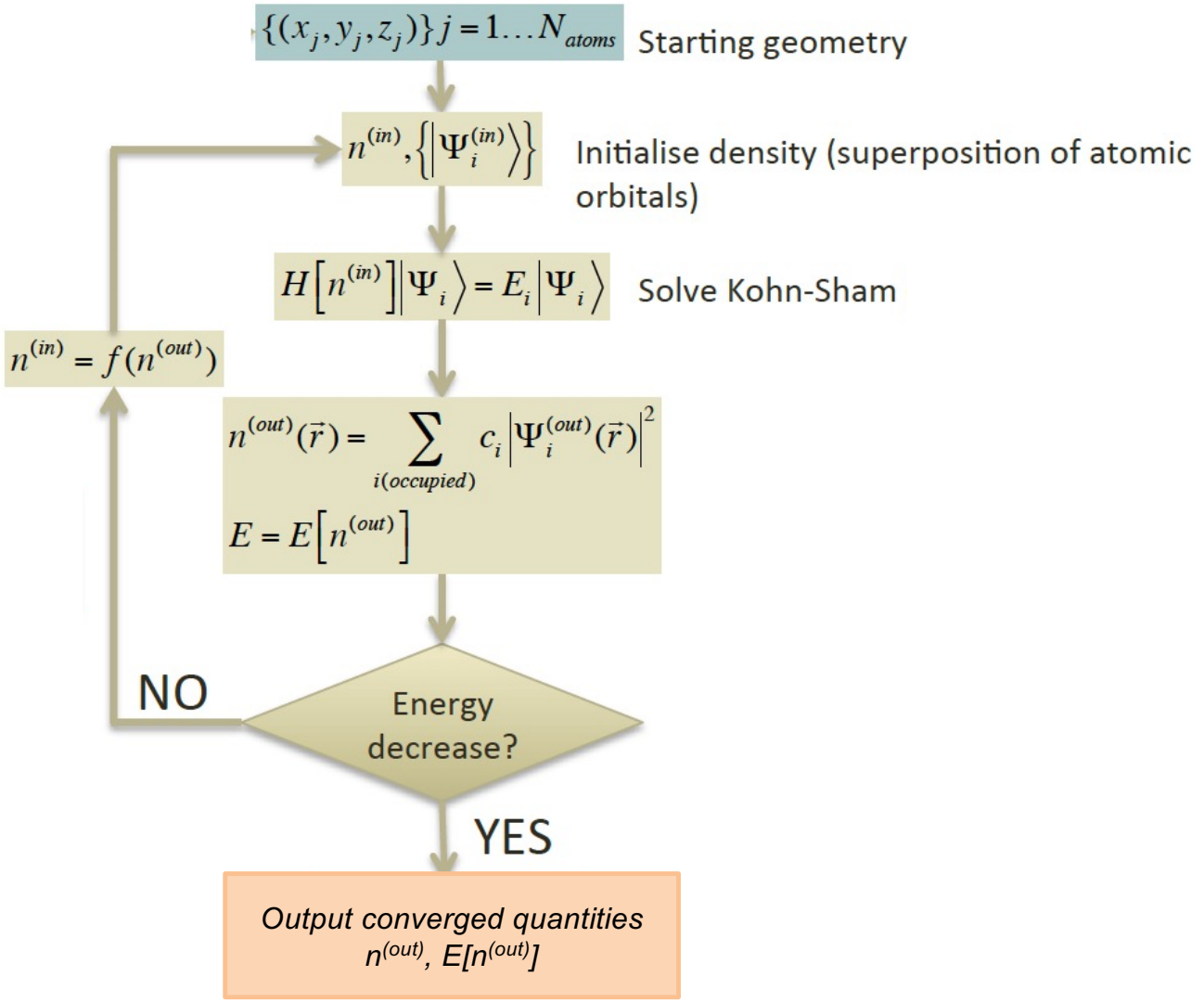


We will explore N-AGNRs with N=7, 10, 13

Note: Edge C atoms are passivated with H

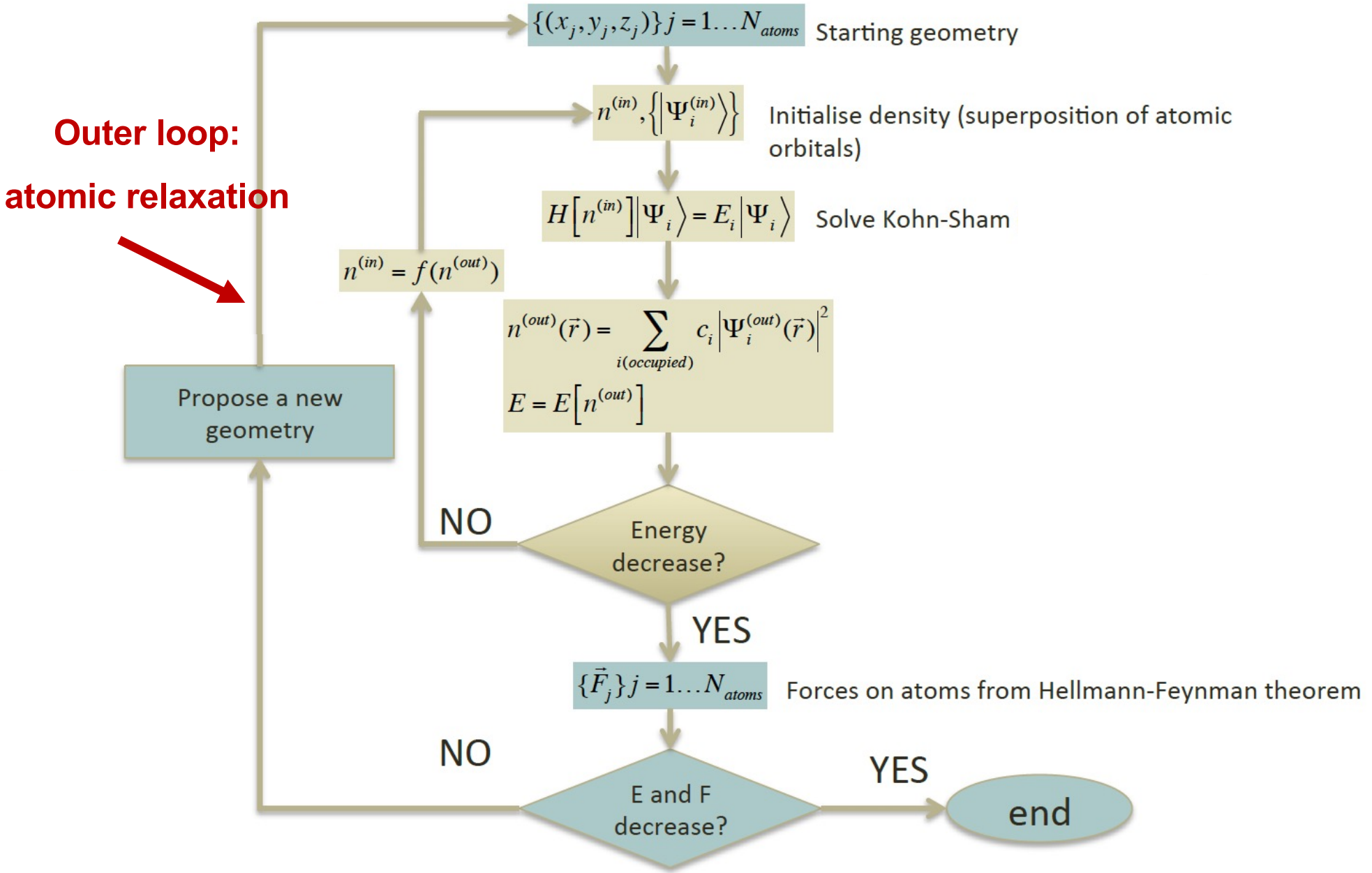
- Which is the most important property of AGNRs?
- What do you expect to observe as N increases?

Typical DFT program flow chart



Source: M. Blanco-Rey (UPV/EHU)

Typical DFT program flow chart



Exercise 2: graphene nanoribbon (1D system)

Go to: **/scratch/esc#/EXERCISE_3_GNR/7AGNR/0_Relaxation**

A geometry optimization will be performed (force minimization)

An “outer loop” is included in the SIESTA calculation

```
###############
#             #
# Relaxation  #
#             #
###############

MD.TypeOfRun CG
MD.MaxForceTol 0.04 eV/Ang
MD.NumCGsteps 1000
```

An additional block must be included in RUN.fdf

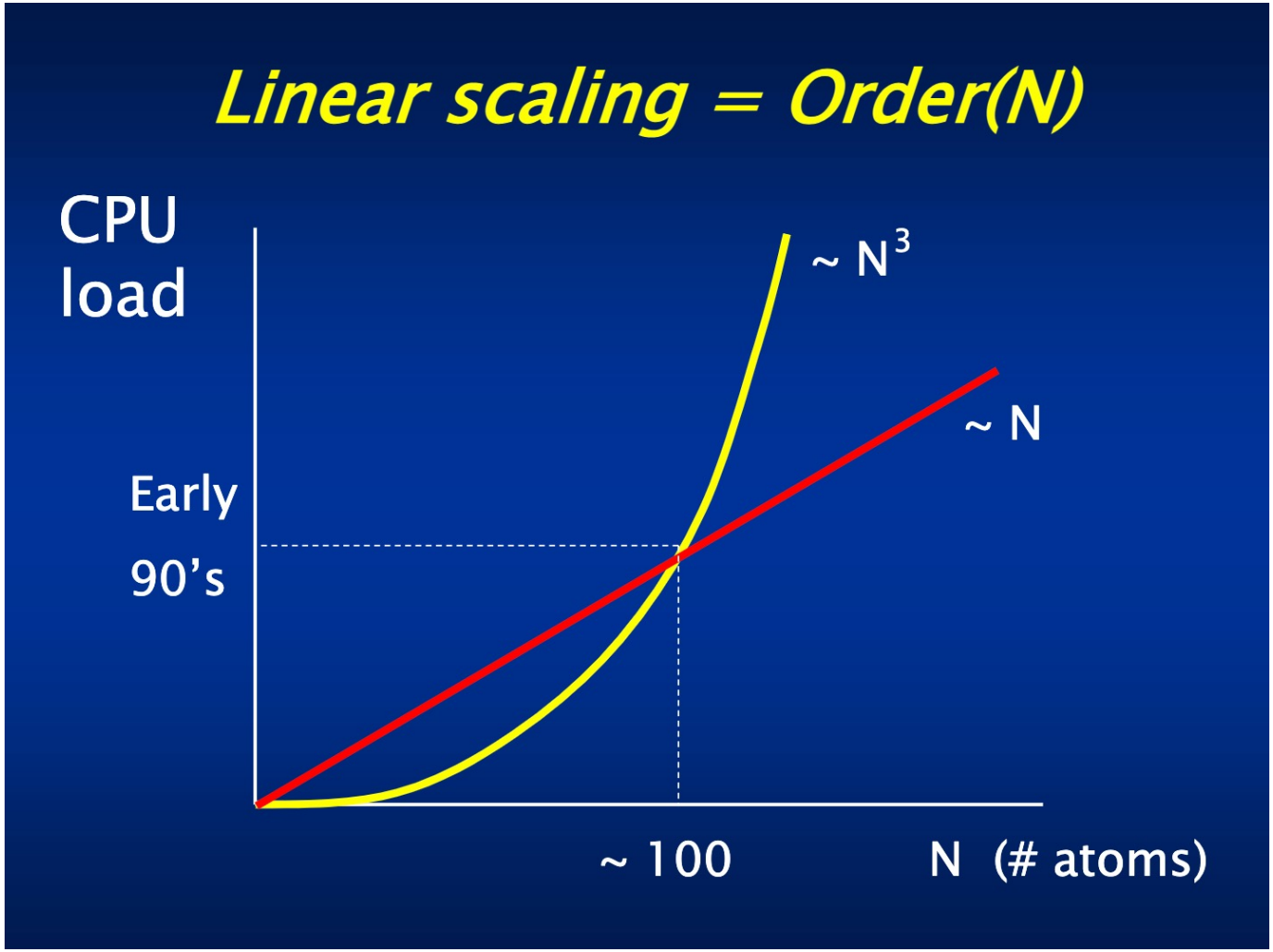
Exercise 2: graphene nanoribbon (1D system)

Go to: **/scratch/esc#/EXERCISE_3_GNR/7AGNR/0_Relaxation**

TODO

- How is the k-grid of a GNR?
- Run Siesta to obtain the relaxed geometry
- What do *7-AGNR.FA* and *7-AGNR.XV* files contain?
- **xv2xsf** can be used to plot the relaxed structure, and **xcrysden** to explore how the C-C bonds have been modified at the edges (with respect to d_{cc}=1.42 Å in extended graphene)
- Repeat the calculation for 10-AGNR and 13-AGNR
- How does the calculation time change with the size of the nanoribbon (*AGNR.XV* files contain?

Exercise 2: graphene nanoribbon (1D system)



Source: P. Ordejón (ICN2)

Exercise 2: graphene nanoribbon (1D system)

Go to: **/scratch/esc#/EXERCISE_3_GNR/7AGNR/1_Banstructure_DOS**

A post-processing calculation to obtain the electronic band structure and DOS

TODO

- Define the Brillouin zone and high-symmetry direction of an AGNR
- Run a single point calculation (no relaxation), adding the required blocks for the band structure and DOS
- Plot the band structure and DOS for the 3 considered nanorribons, and compare the results. How does the band gap change?

Exercise 2: graphene nanoribbon (1D system)

Go to: **/scratch/esc#/EXERCISE_3_GNR/7AGNR/2_Frontier_Bands**

A post-processing calculation to obtain the frontier bands

Electronic bands lying closest to Fermi level: valence (VB) and conduction (CB) bands

An additional block must be included in RUN.fdf

```
##################
#                #
# Wavefunction   #
#                #
##################

Write.Denchar   T
%block WaveFuncKPoints
0.0 0.0 0.0  from iorb_VB to iorb_CB
%endblock WaveFuncKPoints
```

Orbital indexes for VB and CB must be identified in 7-AGNR.EIG

Exercise 2: graphene nanoribbon (1D system)

Go to: **/scratch/esc#/EXERCISE_3_GNR/7AGNR/2_Frontier_Bands**

TODO

- What does the *Graphene.selected.WFSX* file contain?
- In order to plot the frontier orbitals, we will make use of the **denchar** SIESTA utilitiy, which requires an input file. Check **input_denchar.mpr** in the corresponding directory, and comment on its content.
- Execute the following:

```
> cp Graphene.selected.WFSX Graphene.WFSX
> denchar < input_denchar.fdf
```

- Which are the output files printed out by **denchar**? Note that at Γ point, the electron wavefunctions must real.
- Employ **xcrysden** to visualize the wavefunctions (*.cube files). Comment on the differences between VB and CB.