# An introduction to TranSIESTA

The voltage sibling of SIESTA

Pol Febrer (ICN2), SIESTA school 2023

**TRANSIESTA LITERATURE**

2003

Comparative Study > Ann N Y Acad Sci. 2003 Dec;1006:212-26. doi: 10.1196/annals.1292.014.

## TranSIESTA: a spice for molecular electronics

Kurt Stokbro [1], Jeremy Taylor, Mads Brandbyge, Pablo Ordejón

Affiliations + expand

PMID: 14976020 DOI: 10.1196/annals.1292.014

---

2016

## Improvements on non-equilibrium and transport Green function techniques: The next-generation TRANSIESTA

Nick Papior [a] ✉, Nicolás Lorente [b, c] ✉, Thomas Frederiksen [c, d] ✉, Alberto García [c] ✉, Mads Brandbyge [a] ✉

[a] Center for Nanostructured Graphene (CNG), Department of Micro- and Nanotechnology (DTU Nanotech), Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

**TRANSIESTA LITERATURE**

2003

Comparative Study > Ann N Y Acad Sci. 2003 Dec;1006:212-26. doi: 10.1196/annals.1292.014.

## TranSIESTA: a spice for molecular electronics

**TranSIESTA ≠ transport**

2016

## Improvements on non-equilibrium and transport Green function techniques: The next-generation TRANSIESTA

Nick Papior [a], Nicolás Lorente [b, c], Thomas Frederiksen [c, d], Alberto García [c], Mads Brandbyge [a]

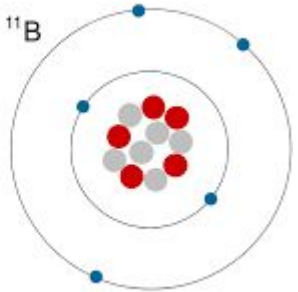
[a] Center for Nanostructured Graphene (CNG), Department of Micro- and Nanotechnology (DTU Nanotech), Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

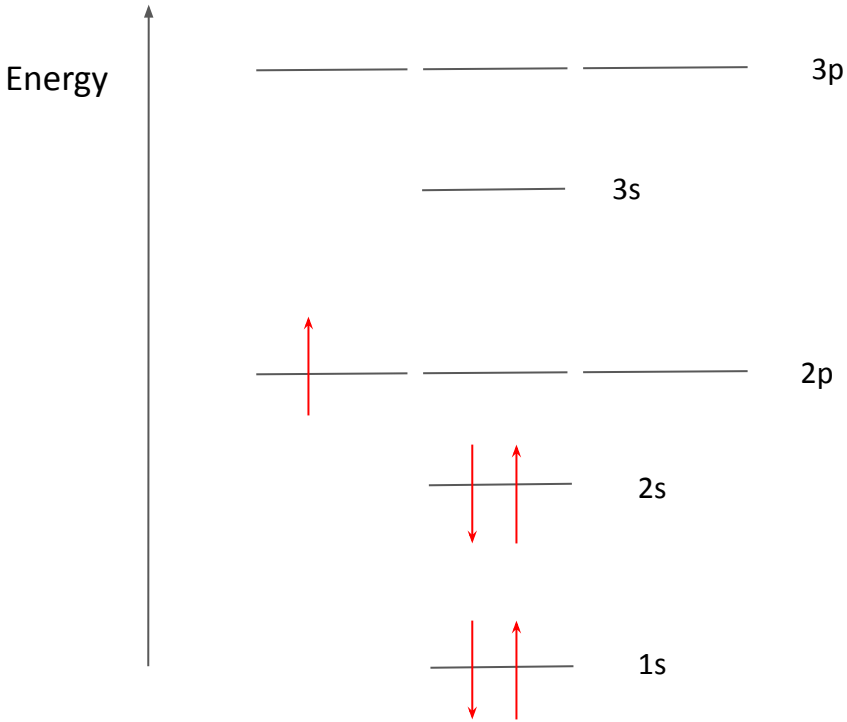
# Why is TranSIESTA needed?

Couldn’t plain old SIESTA have a voltage input?

# “USUAL” WAY TO SOLVE ELECTRONIC DENSITIES

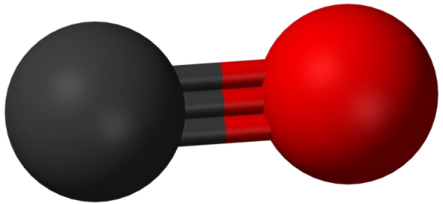
Electronic levels of an atom

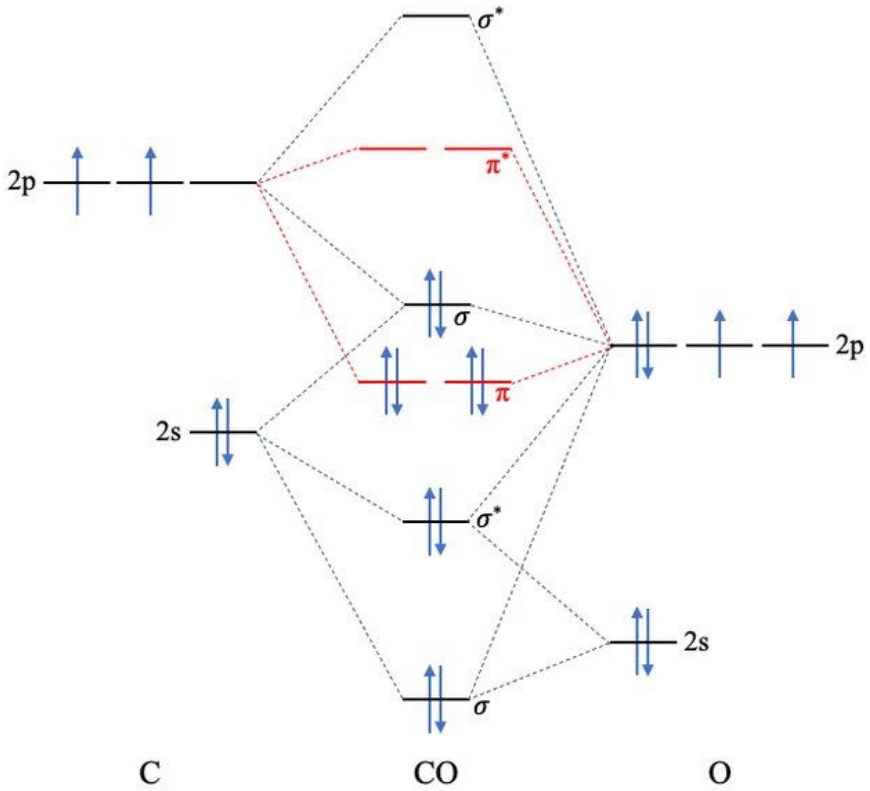


## “USUAL” WAY TO SOLVE ELECTRONIC DENSITIES

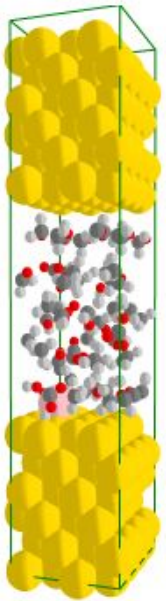
Electronic levels of a molecule



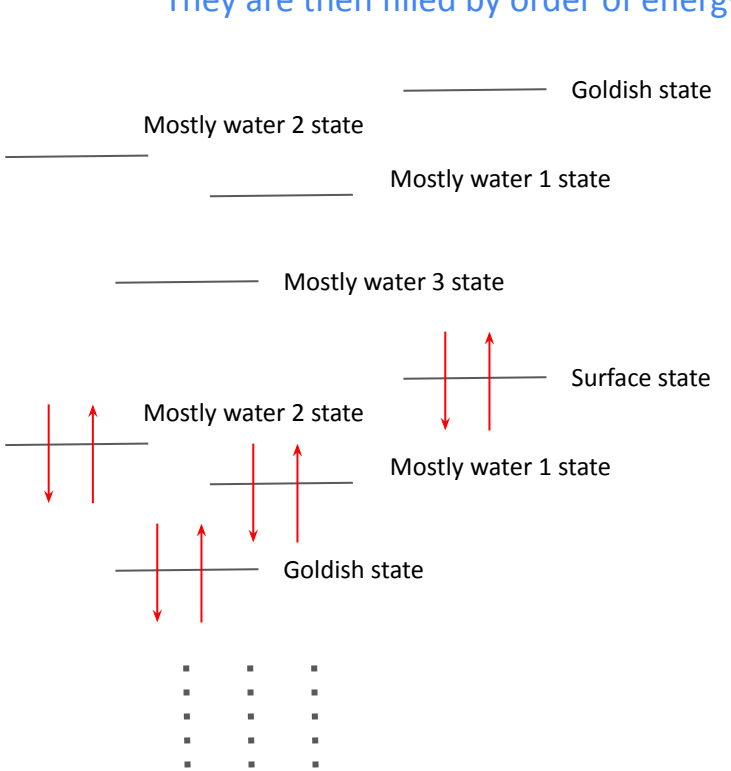


# “USUAL” WAY TO SOLVE ELECTRONIC DENSITIES

Electronic levels of a DFT unit cell



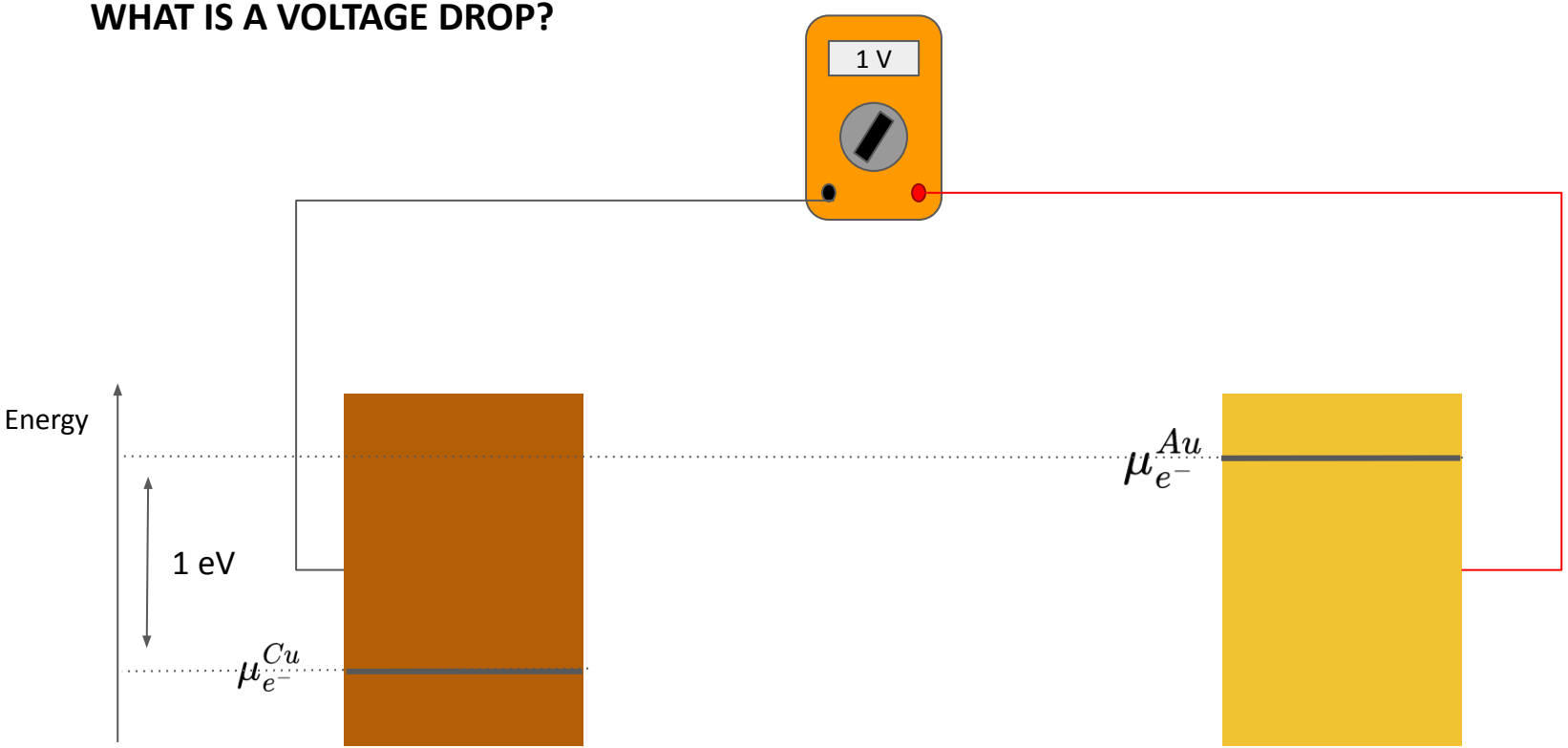
States are combinations of ALL atoms.
They are then filled by order of energy.



## “USUAL” WAY TO SOLVE ELECTRONIC DENSITIES

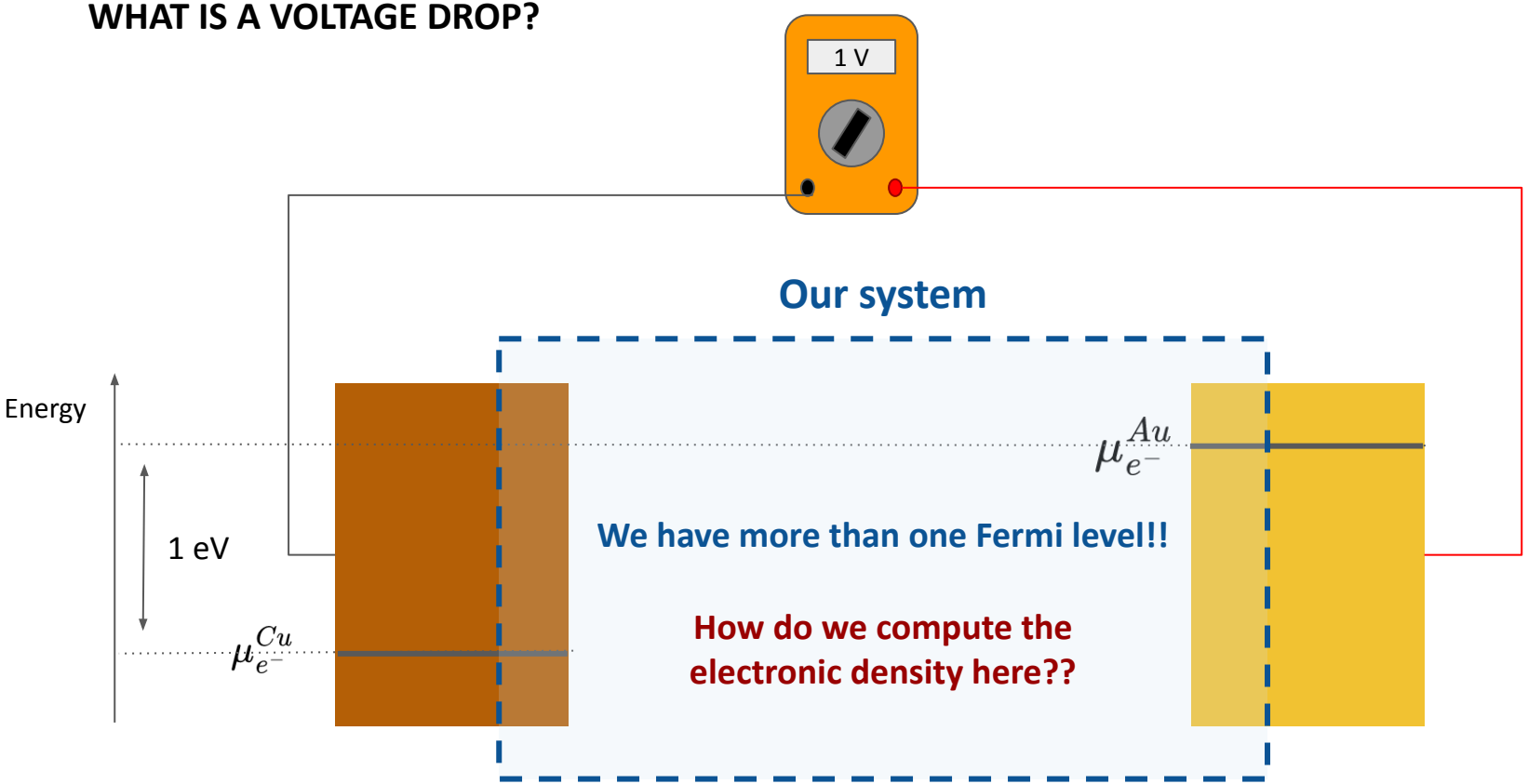
We fill states up until the **Fermi level**.

# WHAT IS A VOLTAGE DROP?




When you apply voltage, you create a **difference in fermi levels**.

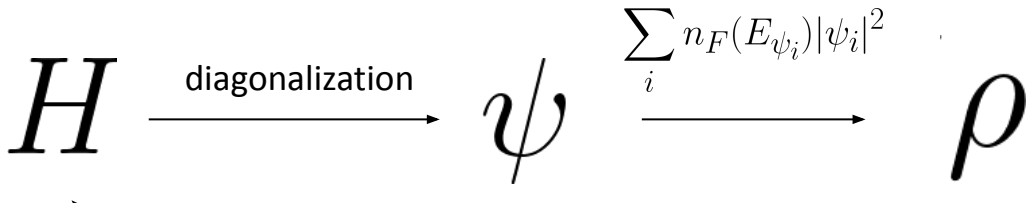
## WHAT IS A VOLTAGE DROP?

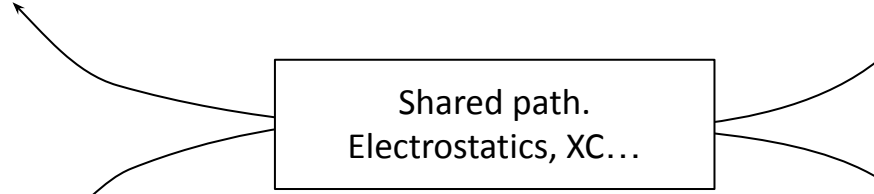



When you apply voltage, you create a **difference in fermi levels**.

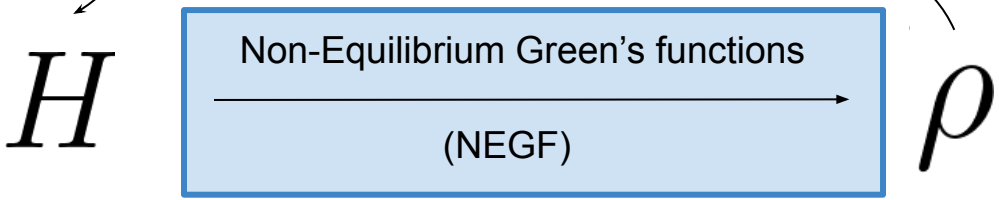
**FROM HAMILTONIAN TO ELECTRONIC DENSITY.**

A single fermi level:



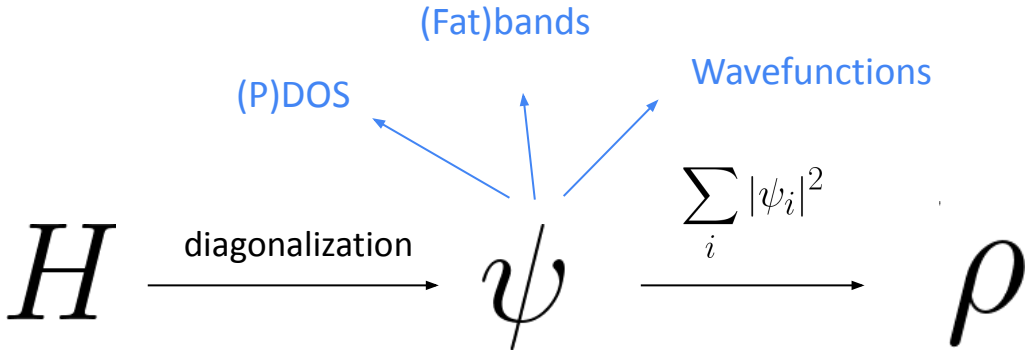

Multiple Fermi levels:



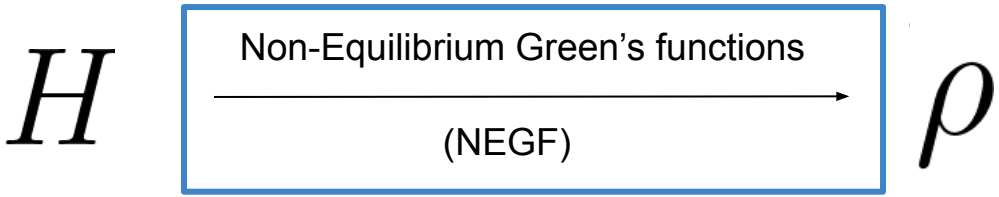

**This is what we know as TranSIESTA**

**POSTPROCESSING.**

A single fermi level:



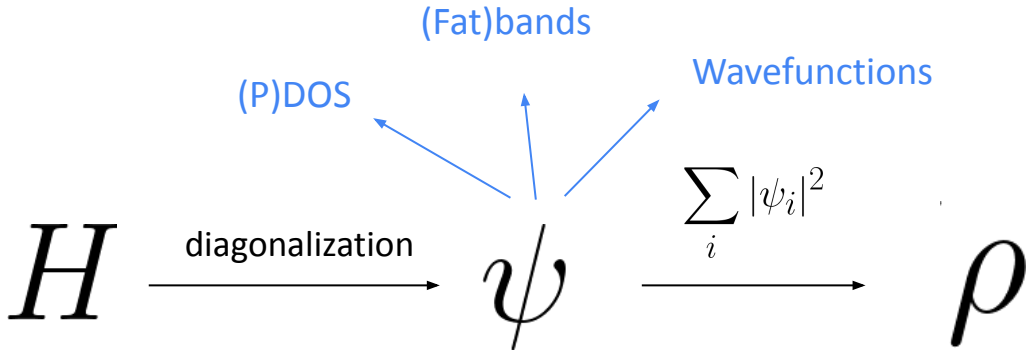

Multiple Fermi levels:



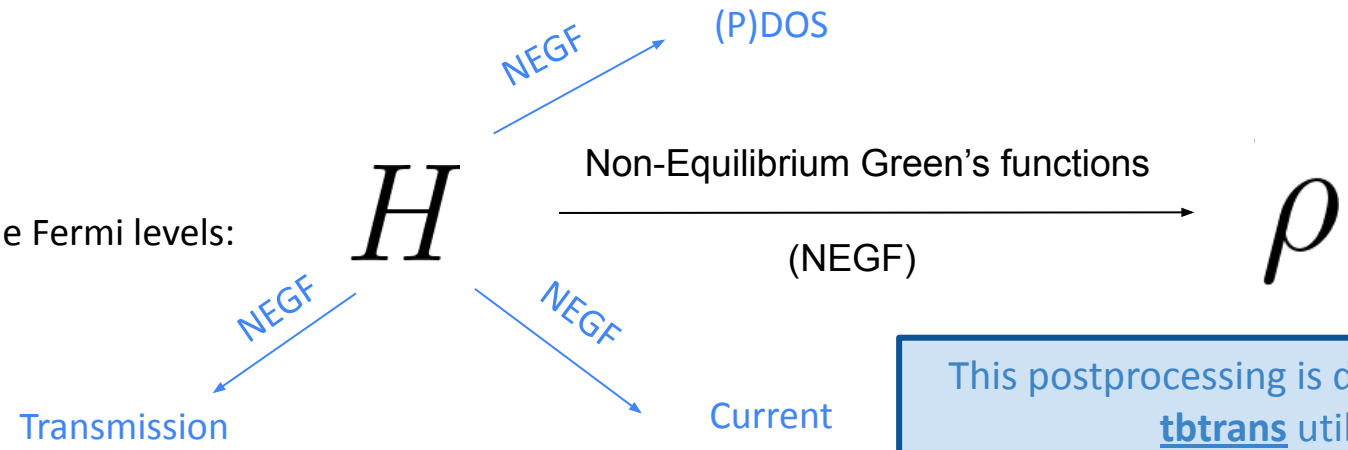

**What do we do if we don't have eigenstates??**

**POSTPROCESSING.**

A single fermi level:

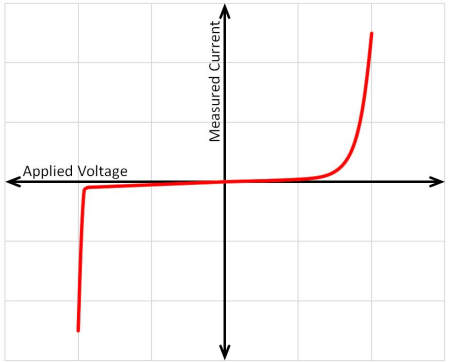



Multiple Fermi levels:




This postprocessing is done with the **tbtrans** util.

# Where do I click to get the I(V) curve?

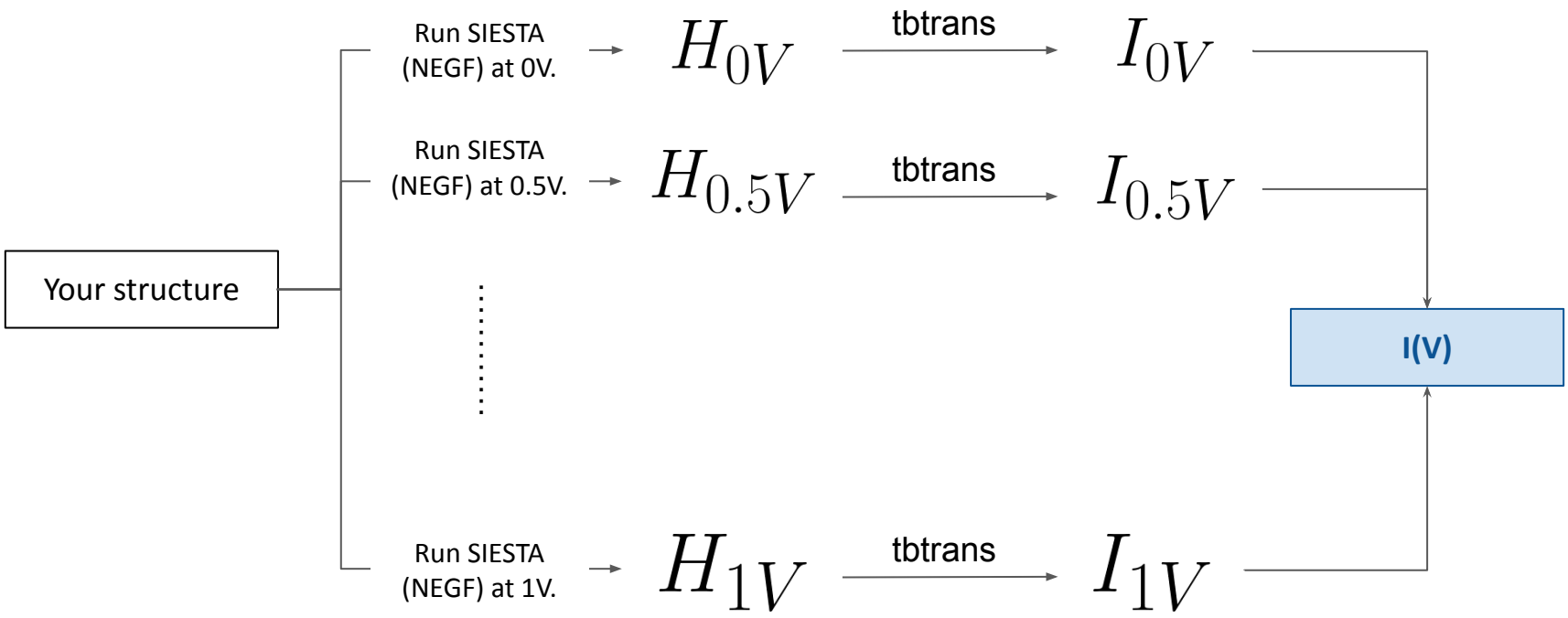



The question everyone asks.

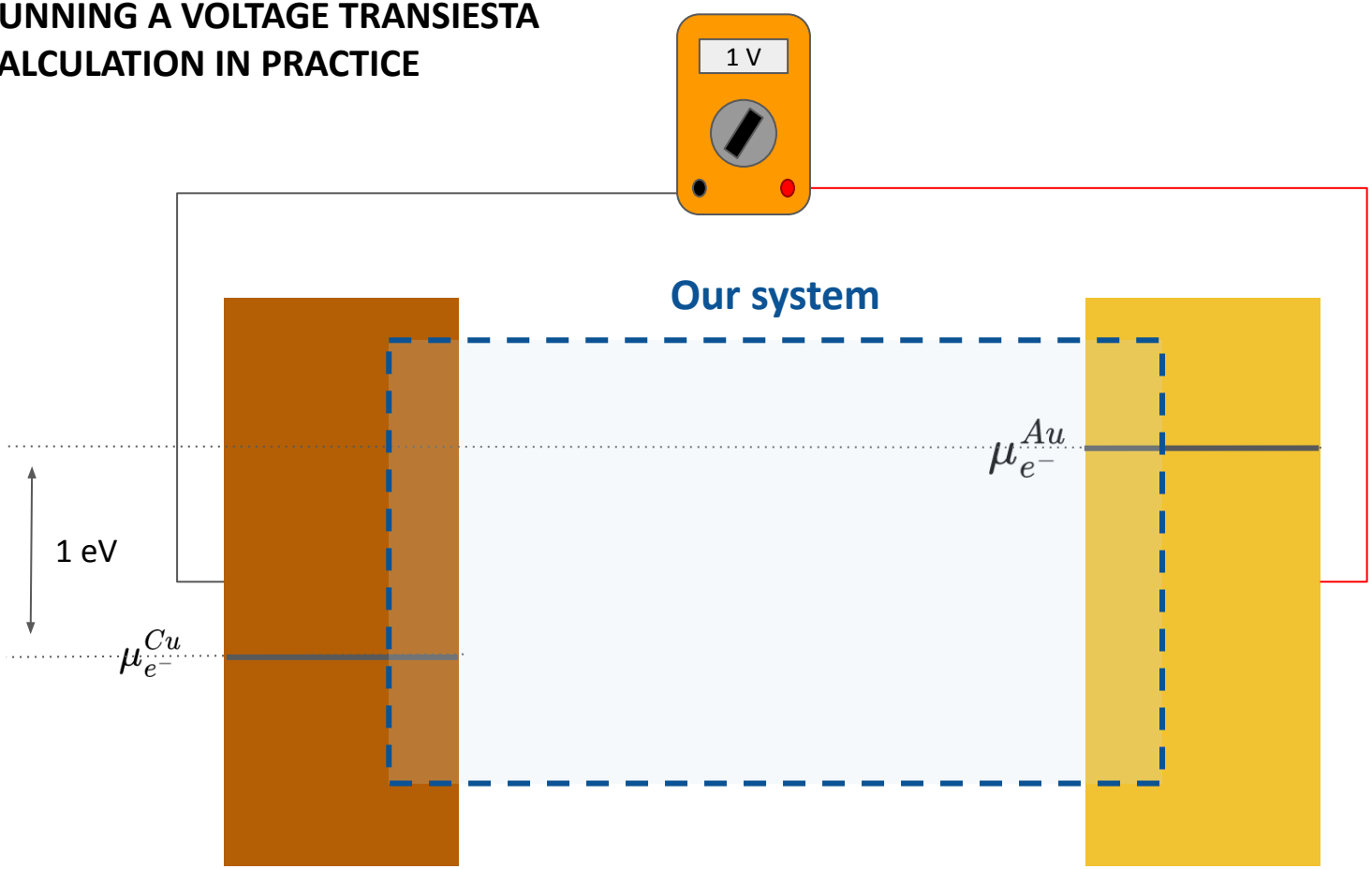
# Where do I click to get the I(V) curve?

There’s no magic button!

## PLOTTING AN I(V) CURVE

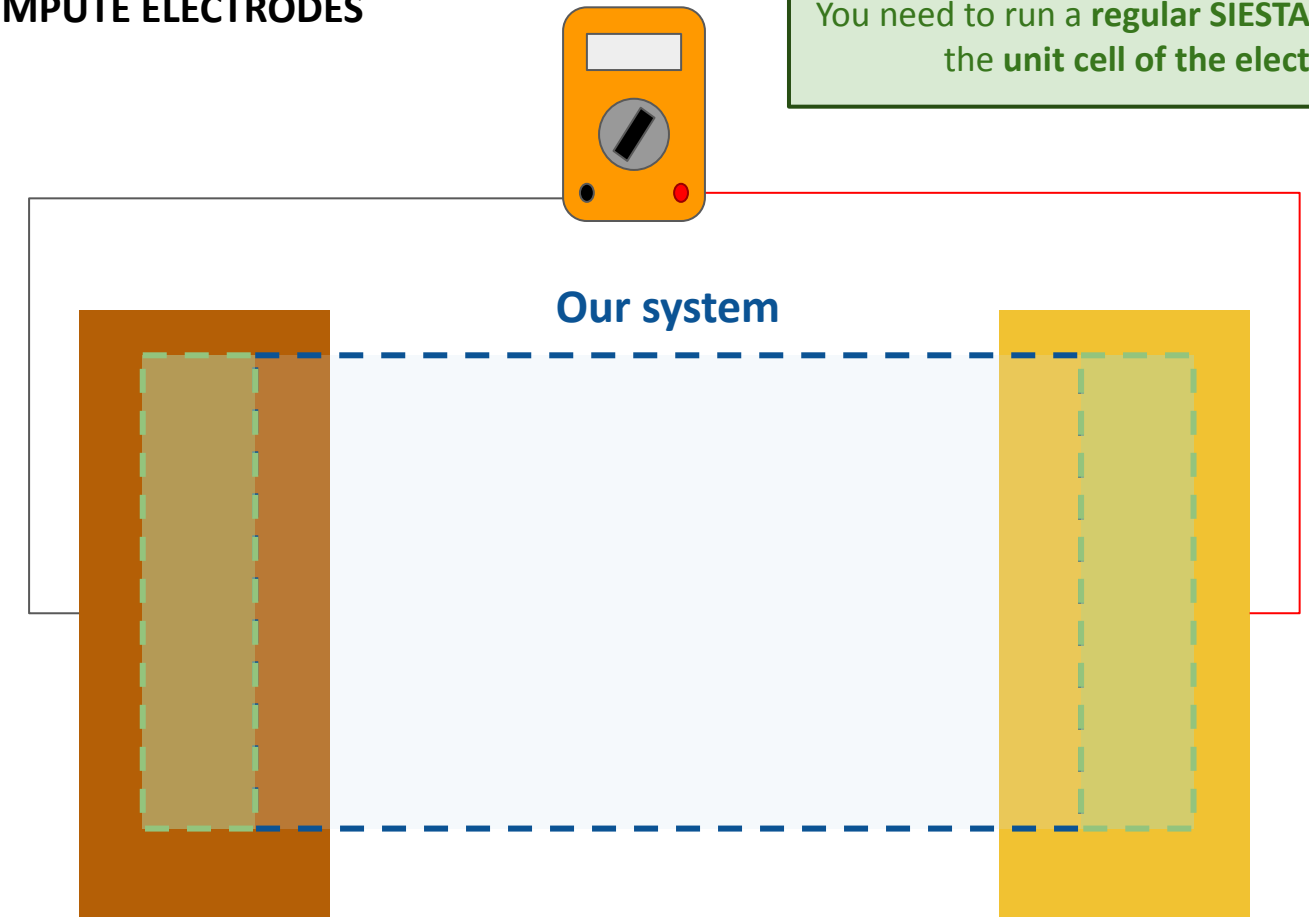


## RUNNING A VOLTAGE TRANSIESTA CALCULATION IN PRACTICE



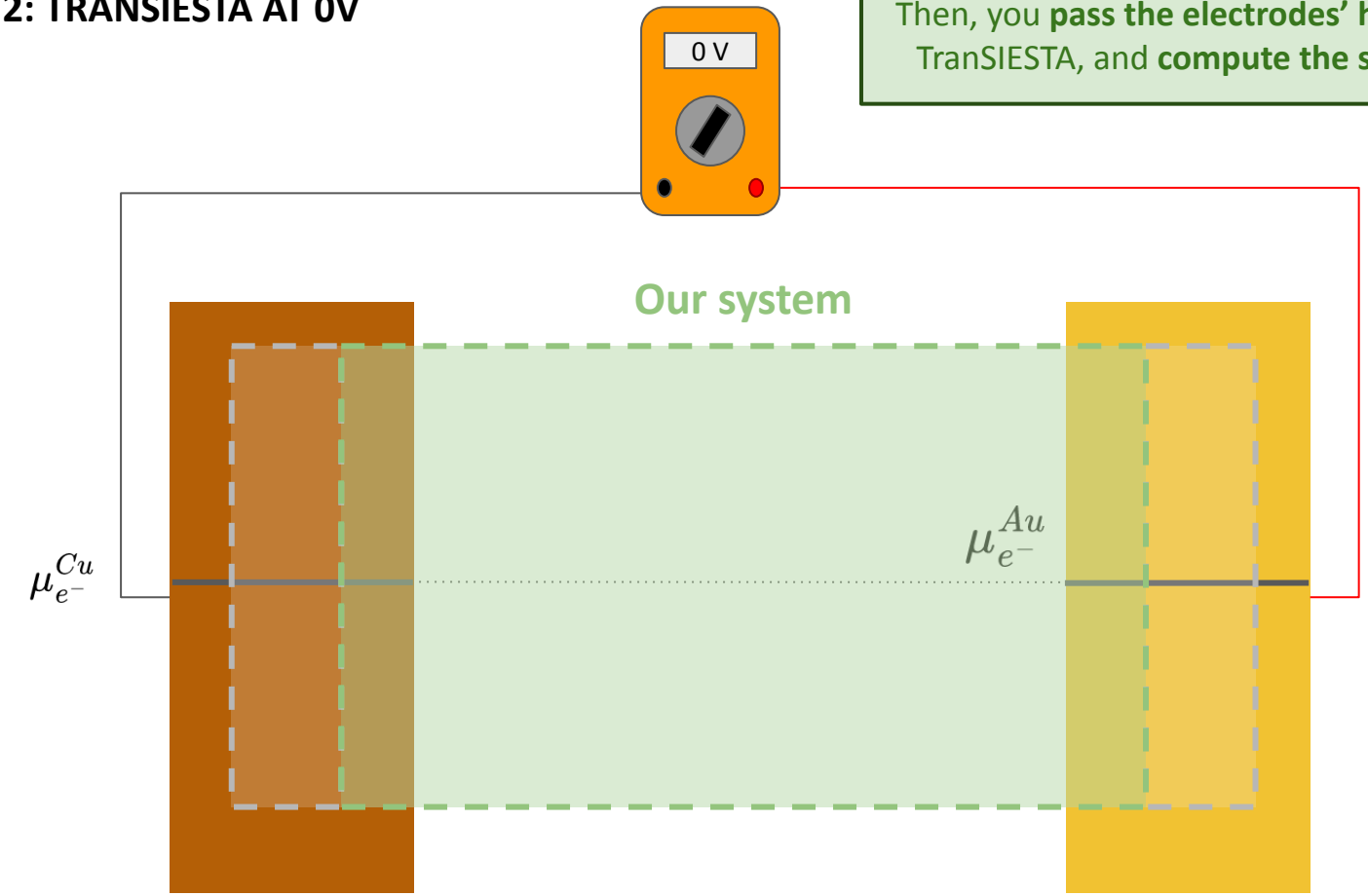
## STEP 1: COMPUTE ELECTRODES

You need to run a **regular SIESTA** calculation for the **unit cell of the electrodes**.



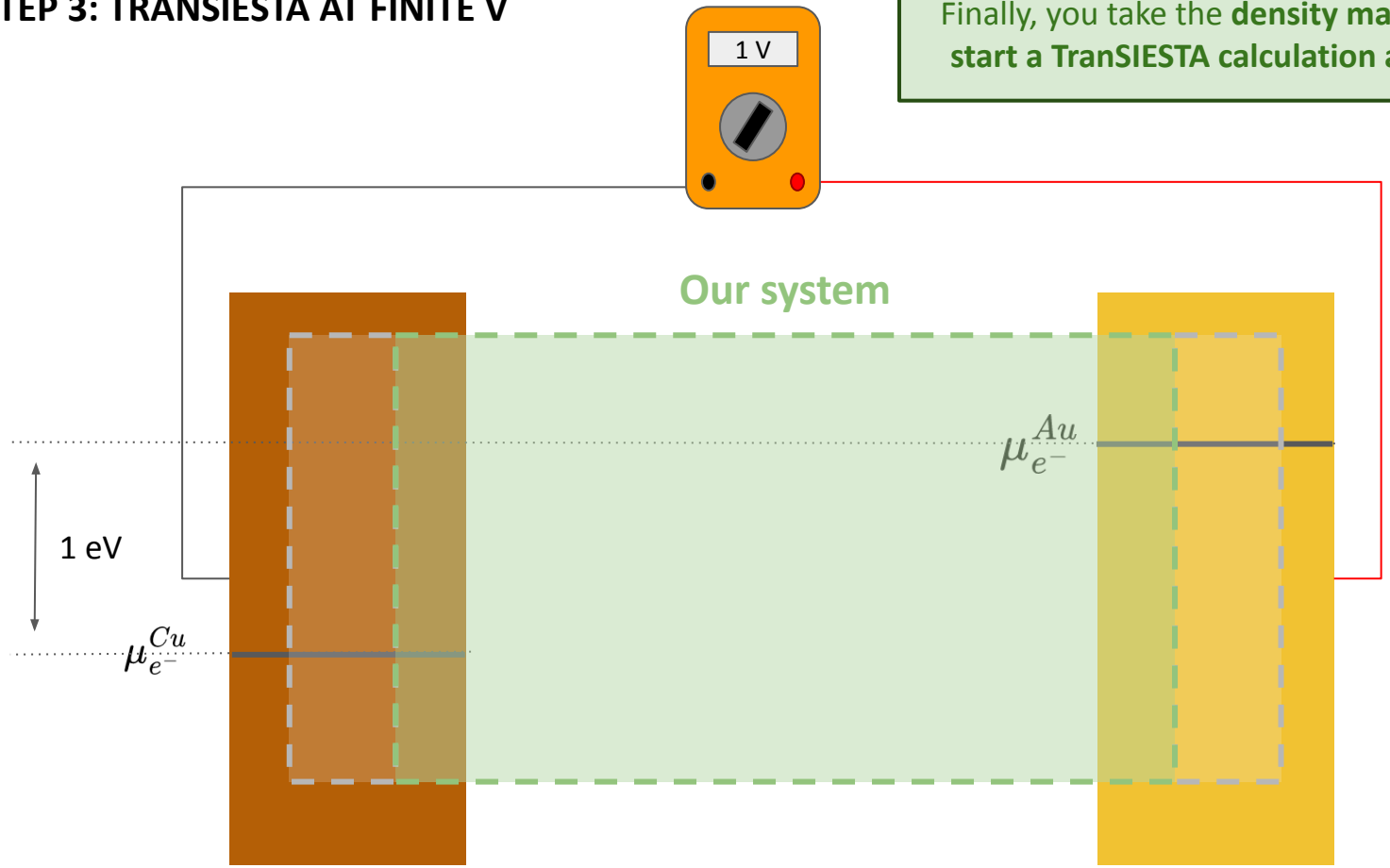
## STEP 2: TRANSIESTA AT 0V

Then, you **pass the electrodes' hamiltonian** to TranSIESTA, and **compute the system at 0V**.



## STEP 3: TRANSIESTA AT FINITE V

Finally, you take the **density matrix at 0V** and **start a TranSIESTA calculation at 1V from it**.

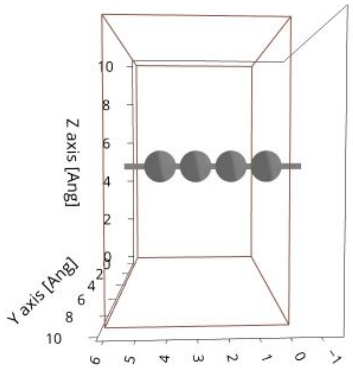


## RUNNING A VOLTAGE TRANSIESTA CALCULATION IN PRACTICE

1. Compute electrodes with SIESTA.
2. Compute system with TranSIESTA at 0V.
3. Compute system with TranSIESTA at finite voltage.

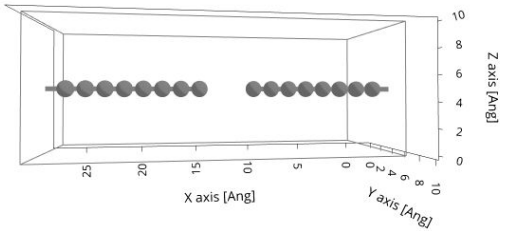
**THE HANDS ON**

Our electrode:



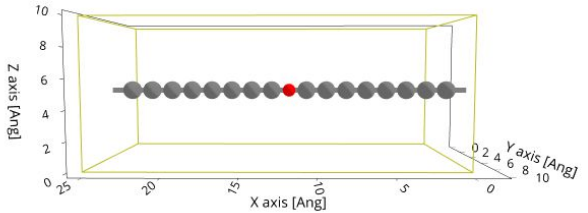

A 1D carbon chain along X.

## Part 1: Compute PDOS at 0V and 1V.




Unconnected chains.

## Part 2: Compute an I(V) curve.




Chains connected by an O atom.