Structure setup for TranSIESTA calculations

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Tel Aviv SIESTA/TranSIESTA workshop

10. September 2014

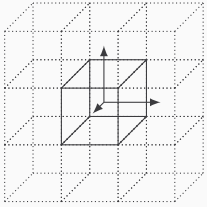
Outline

TranSIESTA setup vs. SIESTA setup

Periodicity

SIESTA

- Fully periodic in 3 (all) cell directions
- Periodicity handled by k-points



TranSIESTA setup vs. SIESTA setup

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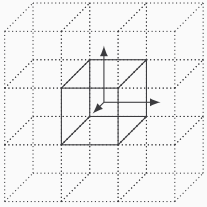
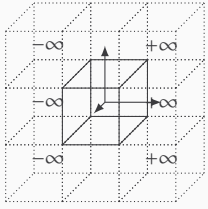
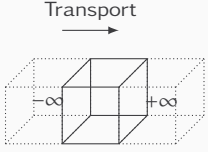


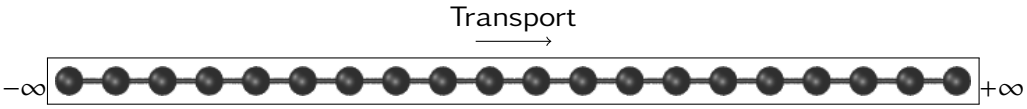
TranSIESTA

- Periodic in 2 cell directions
- Periodicity handled by k-points
- Semi-infinite in 1 cell direction
- Semi-infinite directions handled by self-energies (Σ)



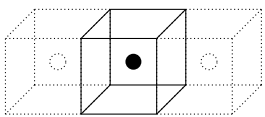


The perfect chain

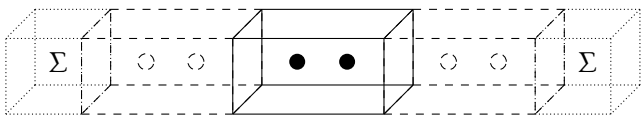


- Perfect systems can be handled equivalently, yet with different methods
- However, SIESTA is the best method for fully periodic systems when *not* applying a bias

SIESTA $k \to \infty$



TranSIESTA $k = 1$



Left Device / Right
Scattering region

The electrodes

Semi-infinite — *bulk*

Self-energies Σ, *VERY IMPORTANT*

We utilise the method by Sancho, Sancho, and Rubio, DOI: 10.1088/0305-4608/15/4/009 which is an iterative scheme for calculating the bulk/surface self energies.

- It requires only principal cell interactions

$$\begin{bmatrix} \mathbf{H}_{00} & \mathbf{H}_{01} & 0 & \dots & \\ \mathbf{H}_{10} & \mathbf{H}_{11} & \mathbf{H}_{12} & 0 & \dots \\ 0 & \mathbf{H}_{21} & \mathbf{H}_{22} & \mathbf{H}_{23} & \ddots \\ \vdots & 0 & \ddots & \ddots & \ddots \end{bmatrix}$$

- Sets a lower boundary on cell size in transport direction
- No limitation on two other direction cell sizes
- High k-point sampling in transport direction and same k-point sampling in transverse directions

Electrodes

Your first setup

1. An electrode is a *pure* SIESTA calculation with a high number of k-points in the transport direction.
   - Why is that?

3. Solve it with `SolutionMethod diagon` using the `transiesta` executable (we only use `transiesta` to get the TSHS-file)
4. Ensure only principal cell interactions! (*see WARNING in output*)
5. Same k-point sampling in the transverse directions *are* required

Electrodes

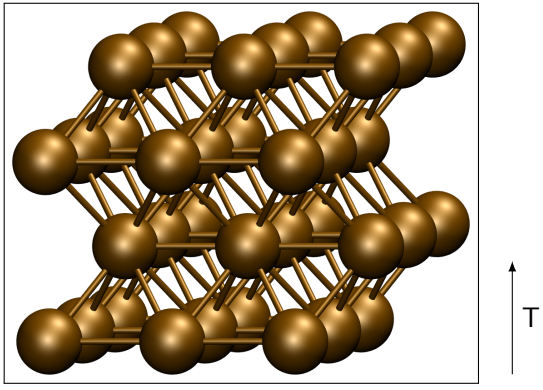
Your first setup

1. An electrode is a *pure* SIESTA calculation with a high number of k-points in the transport direction.
2. The structure needs to be periodic in the transport direction
3. Solve it with `SolutionMethod diagon` using the `transiesta` executable (we only use `transiesta` to get the TSHS-file)
4. Ensure only principal cell interactions! (*see WARNING in output*)
5. Same k-point sampling in the transverse directions *are* required

Benzene dithiol (BDT)

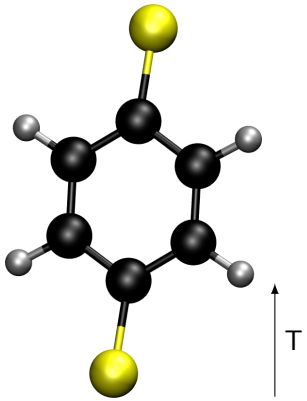
Electrode

- BDT attached to Gold electrodes
- We utilise 100 surface (AB-stacking)
- Decide k-point sampling in transverse direction (converge)



Benzene dithiol (BDT)

Define the molecule

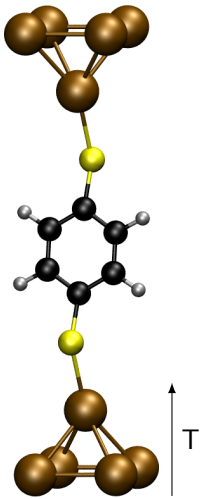


- Relax structure using SIESTA (lecture tomorrow)

Benzene dithiol (BDT)

Intermediate connect

Attach gold connection to the molecule

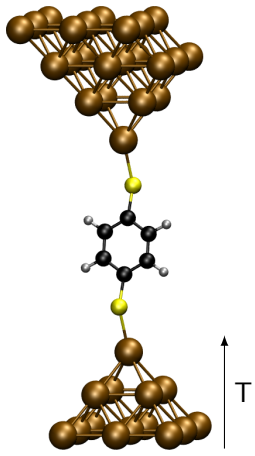


- Consider stacking of *pyramids*
  - A-BDT-A
  - A-BDT-B
  - B-BDT-B
- Relax structure *again,* constrain the *pyramids*

Benzene dithiol (BDT)

Intermediate electrode layers

Attach a couple of electrode layers

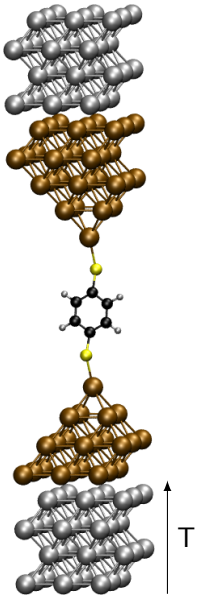


- *Follow* the stacking!
- Relax structure *again,* constrain the *electrode layers*

Benzene dithiol (BDT)

Attach electrode and more intermediate layers

Attach the electrodes on both sides (converge number of intermediate layers)



- *Follow* the stacking!
- Relax structure *again*, constrain the *electrode layers*
- Determining the extra number of layers:
  - Consider the molecule as a "defect"
  - The defect has a screening length in the central region (the extra electrode layers)
  - Ensure that the electrodes "behave as bulk" electrodes (away from defect)

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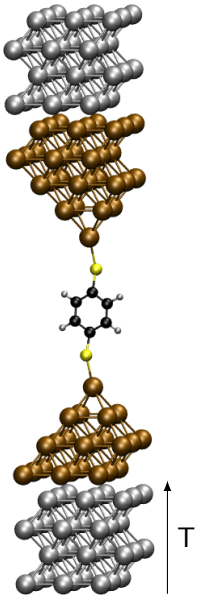

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- What does a metallic electrode require:
  1. Bad screening → many electrode layers
  2. Good screening → few electrode layers
- What does a semi-conducting electrode require:
  1. Bad screening → many electrode layers
  2. Good screening → few electrode layers

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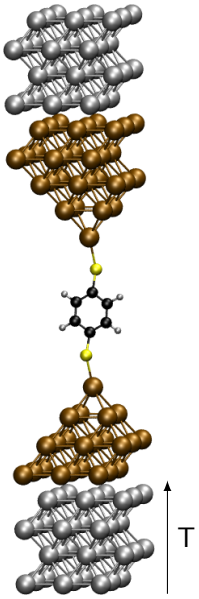

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  2. Good screening → few electrode layers

Structure setup

Electrodes (yes you can use the same electrodes on *both* sides)

```
%block AtomicCoordinatesAndAtomicSpecies
   0. 0. 0.00  1  # 1
   0. 0. 1.42  1  # 2
   0. 0. 2.84  1  # 3
   0. 0. 4.26  1  # 4
%endblock AtomicCoordinatesAndAtomicSpecies
```

System, *always* consecutive

```
%block AtomicCoordinatesAndAtomicSpecies
   0. 0.  0.00  1 #  1
   0. 0.  1.42  1 #  2
   0. 0.  2.84  1 #  3
   0. 0.  4.26  1 #  4
   0. 0.  5.68  1 #  5
   0. 0.  7.10  1 #  6
   0. 0.  8.52  1 #  7
   0. 0.  9.94  1 #  8
   0. 0. 11.36  1 #  9
   0. 0. 12.78  1 # 10
   0. 0. 14.20  1 # 11
   0. 0. 15.62  1 # 12
   0. 0. 17.04  1 # 13
   0. 0. 18.46  1 # 14
   0. 0. 19.88  1 # 15
   0. 0. 21.30  1 # 16
%endblock AtomicCoordinatesAndAtomicSpecies
```

Left electrode

Device

Right electrode

```
# Define the left electrode
TS.HSFileLeft  elec/siesta.TSHS
# Define the right electrode
TS.HSFileRight elec/siesta.TSHS
# any relative paths are usable
```

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   0. 0.  0.00  1 #  1
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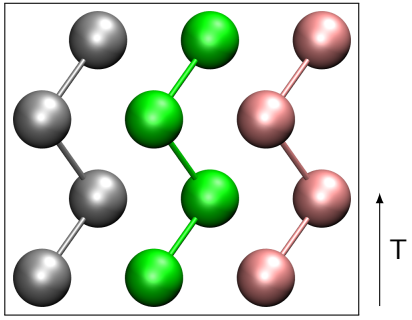
Electrodes using Bloch's theorem

- In case the electrode has simple periodicity in the transverse direction it is encouraged to utilise Bloch's theorem to reduce electrode size



- Requires number of repeated times larger Monkhorst-Pack grid in each direction
- Faster calculation time of electrodes
- Heavily reduces computation time of self-energies

```
# first unit-cell vector
TS.ReplicateLeftA1 3
# second unit-cell vector
TS.ReplicateLeftA2 3
```

Reducing self-energy region

For short orbital range, and atomic plane stacking creates long electrode we can reduce self-energy region (a stacking of ABAB with short orbital cutoff is a good candidate!)

```
TS.NumUsedAtomsLeft  3
TS.NumUsedAtomsRight 3
```

Electrodes (yes you can use the same electrode on *both* sides)

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%block AtomicCoordinatesAndAtomicSpecies
   0. 0. 0.00  1  # 1
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%endblock AtomicCoordinatesAndAtomicSpecies
```

```
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   0. 0.  0.00  1 #  1   } Left electrode
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   0. 0.  2.84  1 #  3   }
   0. 0.  4.26  1 #  4   }
   0. 0.  5.68  1 #  5   }
   0. 0.  7.10  1 #  6   }
   0. 0.  8.52  1 #  7   }
   0. 0.  9.94  1 #  8   } Device
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For short orbital range, and atomic plane stacking creates long electrode we can reduce self-energy region (a stacking of ABAB with short orbital cutoff is a good candidate!)

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The order is determined by the attached orientation

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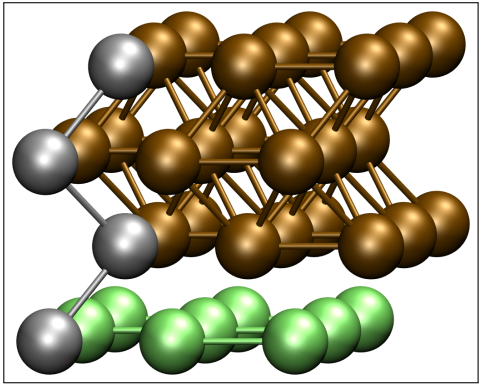
```

Electrode – All together

A short orbital cutoff, long stacking order, Bloch's theorem applicable

```
# Contains the silver atoms:
TS.HSFileLeft ../ELEC/siesta.TSHS
TS.ReplicateLeftA1  3
TS.ReplicateLeftA2  3
# Do not use the green atoms:
TS.NumUsedAtomsLeft 3
```

```
# Contains the silver atoms:
TS.HSFileRight ../ELEC/siesta.TSHS
TS.ReplicateRightA1  3
TS.ReplicateRightA2  3
# Do not use the green atoms:
TS.NumUsedAtomsRight 3
```



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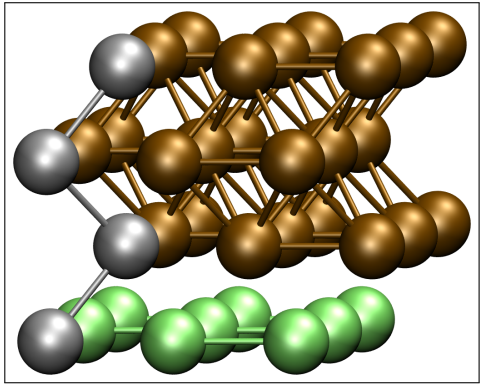

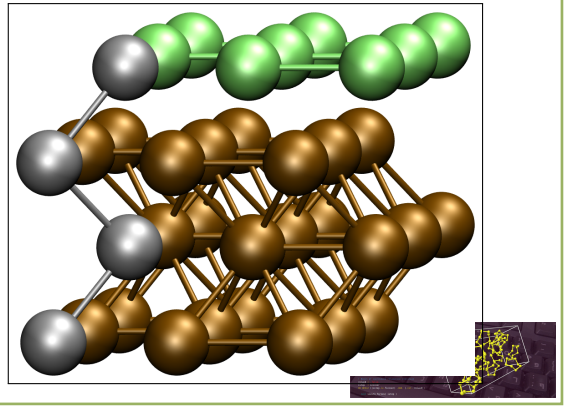

FDF flags

- SolutionMethod diagon/transiesta
- %block AtomicCoordinatesAndAtomicSpecies
- TS.HSFileLeft
- TS.ReplicateLeftA1/TS.ReplicateLeftA2
- TS.NumUsedAtomsLeft
- TS.HSFileRight
- TS.ReplicateRightA1/TS.ReplicateRightA2
- TS.NumUsedAtomsRight

Doing TranSIESTA calculations:

1. calculate electrodes (`transiesta < elec.fdf | tee elec.out`)
2. solve using (`transiesta < chain.fdf | tee chain.out`)
3. calculate transmission (`tbtrans < chain.fdf | tee chain.tbt-out`)