Lab Exercise II : Huckel-IV

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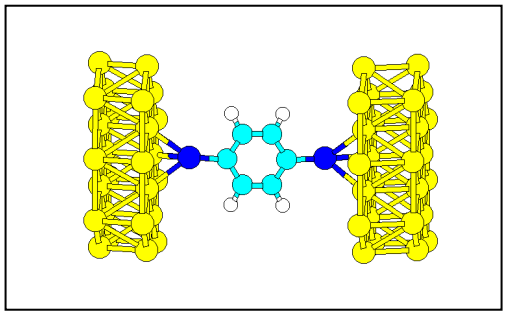
- **Brief Description of Huckel-IV**
- **Huckel-IV on the Hub**
- **Exercises**
- **Few words on Huckel-IV codes**

Brief Description of Huckel-IV

Huckel-IV is a simple semi-empirical model for molecular conduction which can be run from the hub

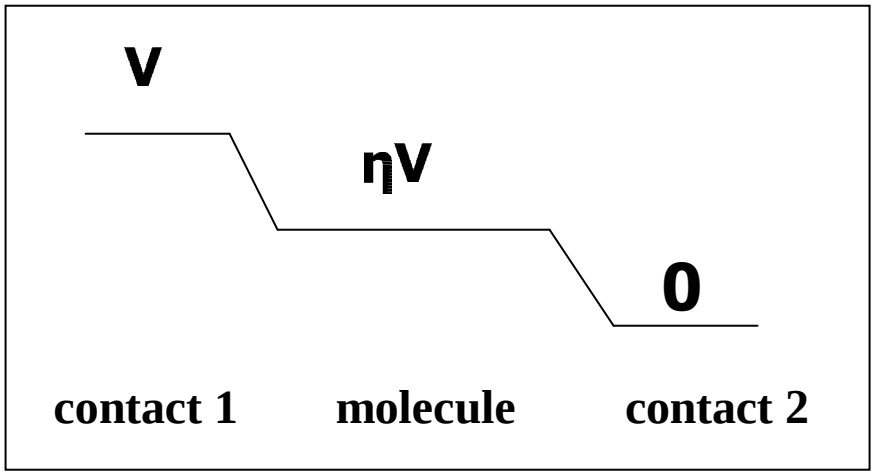
Main features of Huckel-IV are:

- device is modeled by a semi-empirical method : Extended Huckel Theory (EHT)
- Contact is also modeled by EHT and Self energy for the contact is calculated exactly
- System modeled is : gold contact- single molecule-gold contact where the gold surface is in 111 direction
- Model only two terminal device. No gate.



Brief Description of Huckel-IV

- Potential profile inside the molecule is assumed of following shape :



- Two options are provided to the users for the potential calculation : (1) to specify η as a constant and (2) to specify a charging energy U_0 and let the program calculate η(V) self-consistently at each bias.

Brief Description of Huckel-IV

- Potential profile inside molecule is assumed flat in both cases

- The equilibrium Fermi energy (E_F) is treated as a fitting parameter

- The contacts are assumed to have a constant density of states in the energy range of interest

- Structural changes of the molecule under bias are not considered

- A Buttiker type probe is included to simplify calculations

For detailed discussion of the theory of Huckel-IV see:

Ferdows Zahid, Magnus Paulsson and Supriyo Datta,
" Electrical Conduction through Molecules", to appear in forthcoming volume on Advanced Semiconductors and Organic Nano-Techniques, edited by H. Morkoc, Academic Press.
* This article can be obtained from the Huckel-IV main page.

Huckel-IV on the Hub

Huckel-IV is available on Hub

To access Huckel-IV on hub go to: http://nanohub.purdue.edu
and then select ‘Huckle-IV 2.0’

Running a Huckel-IV simulation consists of three stages:

1. Input Stage
2. Execute Stage
3. Output Stage

In the following slides these stages will be briefly discussed

(For more details see the Manual on Huckel-IV main page)

Huckel-IV on the Hub: Main Page

Huckel-IV-Related Information

Description
First Time User's Guide
Manual
Theory of Molecular Conduction
Source
Questions

Run Status

Run Huckel-IV

1. Modify/Create Huckel-IV Input Files
2. Execute Huckel-IV
3. View/Download Huckel-IV Output Files

Huckel-IV on the Hub: Input Stage

- In this stage users will define a coordinate file from the Input page
- Only input required for Huckel-IV is the coordinate file of the molecule
- This coordinate file will specify the structure of the molecule of interest
- This coordinate file should be in ‘XYZ’ format and oriented in proper direction
- Some of the coordinate files can be obtained from the example folder in Huckel-IV Input page
- For other systems users have to generate their own coordinate files using any Chemistry software

Huckel-IV on the Hub: Input Stage

Example of a coordinate file

1	-1.251197	-3.416196	.000000
16	.079083	-3.194823	.000000
6	-.001287	-1.408464	.000000
1	2.152491	-1.227666	.000000
1	-2.156143	-1.223829	.000000
6	1.205002	-.695624	.000000
6	-1.205642	-.697041	.000000
6	-1.205687	.697184	.000000
6	1.204928	.695612	.000000
1	-2.156177	1.224008	.000000
1	2.152382	1.227620	.000000
6	-.001296	1.408515	.000000
16	.079273	3.194817	.000000
1	-1.251173	3.415059	.000000

Atomic number

X coordinate values

Y coordinate values

Z coordinate values

Huckel-IV on the Hub: Input Page

Huckel-IV: Input

Hub Directory | Huckel-IV | Step1:Input | Step2:Execute | Step3:Output

Help for *Step1:Input* | **User:** molecule | **Working Folder:** /huckeliv/Input/

1. Select one of the commands from the categories a, b, c, d, or e.

a.	(•) **Edit File** OR **Open Folder** ( ) **Delete File** OR **Folder** ( ) **Download File to Your Disk**	< *No Files Available* >
b.	( ) **Create New File** ( ) **Create New Sub-Folder**	newname
c.	( ) **Go To Examples Folder**	Working Folder Will Not Change
d.		Commands typed here *override* the check-box selections above.
e.	Browse...	Upload file (*overrides* selections a–d above).

2. Execute the selected command. Execute the Command

Huckel-IV on the Hub: Execute Stage

- In this stage users will run specific simulation by choosing the desired options and parameters in the Execute page

- Five different tasks can be performed

- Task one is independent. Task two has to perform first to do the other three tasks

- Task two is :Build Density of States (DOS) and Transmission Data Files. In this step a data file named ‘Dos_TE.mat’ will be generated. This data file is used for all the calculations for equilibrium and non-equilibrium properties.

[As generating this file is time-consuming (10 minutes to one hour) we will use previously generated ‘Dos_TE.mat’ file for all the calculations in ‘Exercise’ section]

- Details of the steps in Execute page will be discussed in the ‘Exercise’ section with some examples

Huckel-IV on the Hub: Execute Page

Huckel-IV: Execute

Help for *Step2:Execute* | **User:** molecule

Select Task

- (•) Calculate Energy Levels of Neutral Molecule
- ( ) Build Density of States (DOS) and Transmission Data Files
- ( ) Calculate Equilibrium Properties
- ( ) Calculate Non-Equilibrium Properties (Non-Self-Consistent Method)
- ( ) Calculate Non-Equilibrium Properties (Self-Consistent Method)

Next

Hub Directory | Huckel-IV | Step1:Input | Step2:Execute | Step3:Output

Huckel-IV on the Hub: Output Stage

- In this stage users will view the results and plots generated in Execute Stage
- Plots can be generated in both postscript and GIF format
- From the data files users can generate their own plots
- A brief description of all the output data files and plots are given in the ‘Readme’ file in the Output page

Huckel-IV on the Hub: Output Page

Huckel-IV: Output

Hub Directory | Huckel-IV | Step1:Input | Step2:Execute | Step3:Output

Help for *Step3:Output* | **User:** molecule | **Working Folder:** /huckeliv/Output/

1. **Select** one of the commands from the categories a, b, or c.

a.	◉ **View File** OR **Open Folder** ○ **Delete File** OR **Folder** ○ **Download File to Your Disk**	< *No Files Available* >	File Type: Auto
b.	○ **Go To Examples Folder**	Working Folder Will Not Change	
c.		Commands typed here *over-ride* the check-box selections above.	

2. **Execute** the selected command. [Execute the Command]

Exercises

We will perform the following exercises:

- **Exercise-1: To obtain energy levels of neutral phenyl dithiol (PDT)**
  (Purpose of this exercise is to learn how to get the energy levels of neutral molecule)

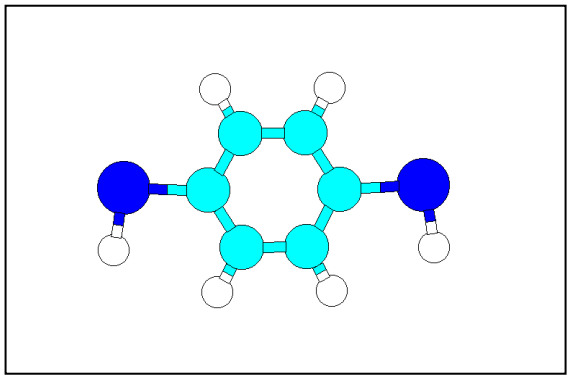
- **Exercise-2: To calculate total Density of States (DOS), Transmission (T) and Charge Neutrality level (E_{cnl}) for PDT connected to two gold contacts**
  (Purpose of this exercise is to see how the contacts affect the energy levels and other properties of a molecule)

- **Exercise-3: To calculate the I-V characteristics of PDT with symmetric coupling**
  (Purpose of this exercise is to see the effect of 'charging' in the I-V characteristics)

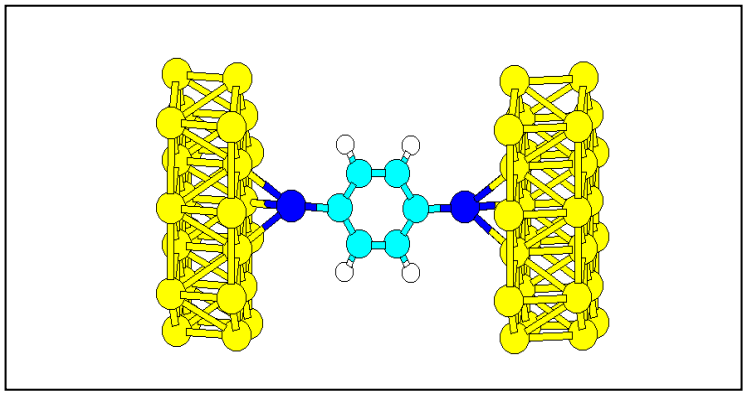
- **Exercise-4: To calculate the I-V characteristics of PDT with asymmetric coupling**
  (Purpose of this exercise is to see the effect of asymmetric coupling in the I-V characteristics)

- **Exercise-5: To calculate the I-V characteristics of Quantum point contact (QPC)**
  (Purpose of this exercise is to see whether we are getting correct result for quantized conductance)

Exercises : Systems

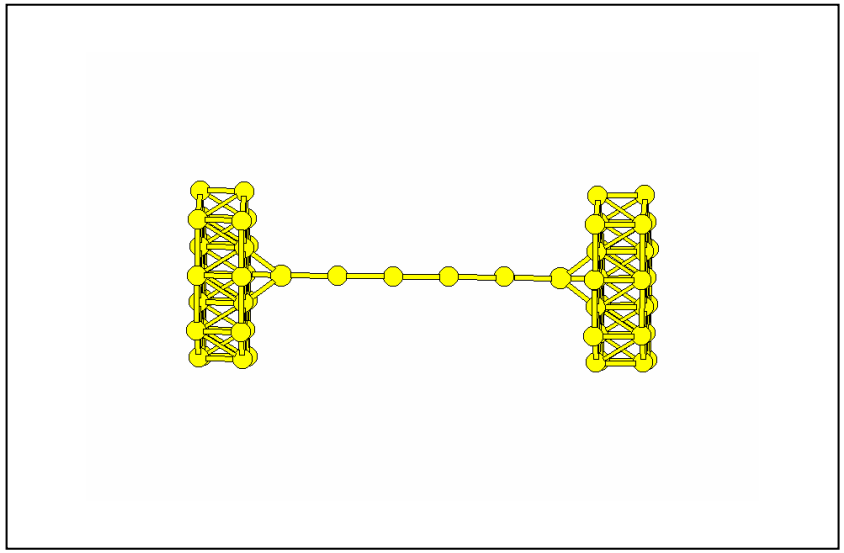


Neutral PDT



PDT connected to gold contacts

QPC connected to gold contacts



Exercise -1 : Procedure

- First upload the coordinate file of neutral PDT from the example folder in Input page (copy the file pdt.dat from pdt directory)

- Next go to main Execute page and select ‘Calculate Energy Levels of Neutral Molecule’

- From ‘Calculate Energy Levels of Neutral Molecule’ page select the correct coordinate file and then put all other parameter values on the blank space correctly (parameter values can be obtained from the README file in example folder in Input page)

- Next push **Calculate Energy Level** button

- In the ‘Program Status’ page keep pushing **Proceed** button until it says ‘ No Programs Executing’. It will take 20 to 30 seconds to finish.

- Then go to the Output page and view Elevels.gif file

Exercise -1 : Procedure

Huckel-IV: Execute

Hub Directory | Huckel-IV | Step1:Input | Step2:Execute | Step3:Output

Help for *Step2:Execute* | **User:** molecule

Calculate Energy Levels of Neutral Molecule

Coordinate File: pdt.dat

Total Number of Electrons: 42

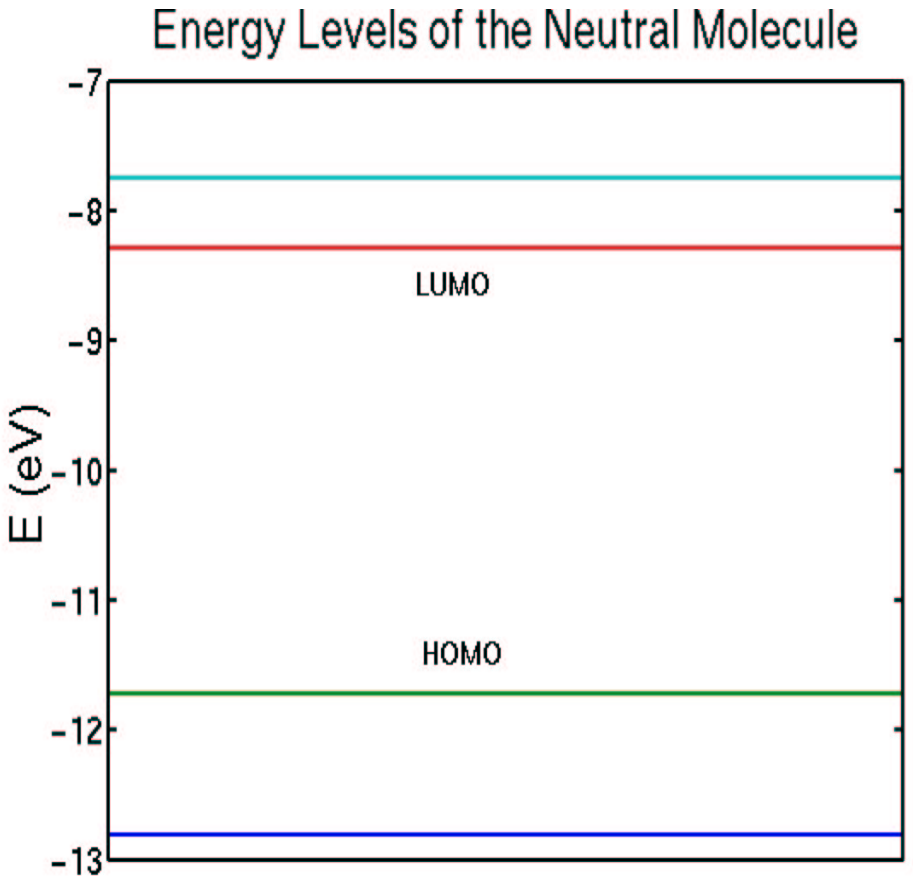
Plot Format(s) *(if any)*

- ☐ GIF (Graphic Interchange Format)
- ☐ PDF (Portable Document Format)
- ☐ PS (PostScript)

Output Folder: pdt

Calculate Energy Level

Exercise -1 : Output



HOMO = -1.7 eV

LUMO = -8.3 eV

HOMO-LUMO gap (HLG) = 3.4 eV

Exercise -2 : Procedure

- First upload the Dos_TE.mat file for PDT from the example folder in Output page (copy the file from pdt directory)

- Next go to main Execute page and select ‘Calculate Equilibrium Properties’

- From ‘Calculate Equilibrium Properties’ page select the Dos_TE.mat file and then put all other parameter values on the blank space correctly
(parameter values can be obtained from the README file in example folder of Input page)

- Next push **Calculate Properties** button

- In the ‘Program Status’ page keep pushing **Proceed** button until it says ‘ No Programs Executing’. It will take 60 to 80 seconds to finish.

- Then go to the Output page and view DOS.gif, TE.gif and E_cnl.gif files

Exercise -2 : Procedure

Calculate Equilibrium Properties

DOS and Transmission Data File: Dos_TE.mat
(from prior step)

Calculate Properties

- [x] Charge Neutrality Level

- [x] Transmission and Density of States

  Energy Grid

  E min: -14

  E max: -6

  dE: 15e-3

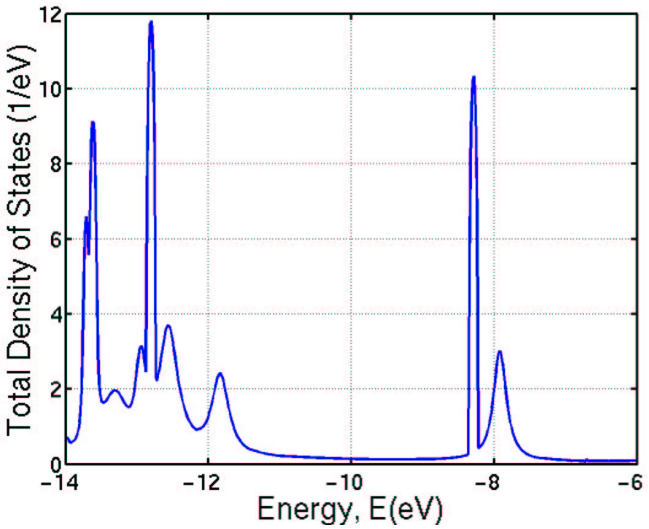
Plot Format(s) *(if any)*

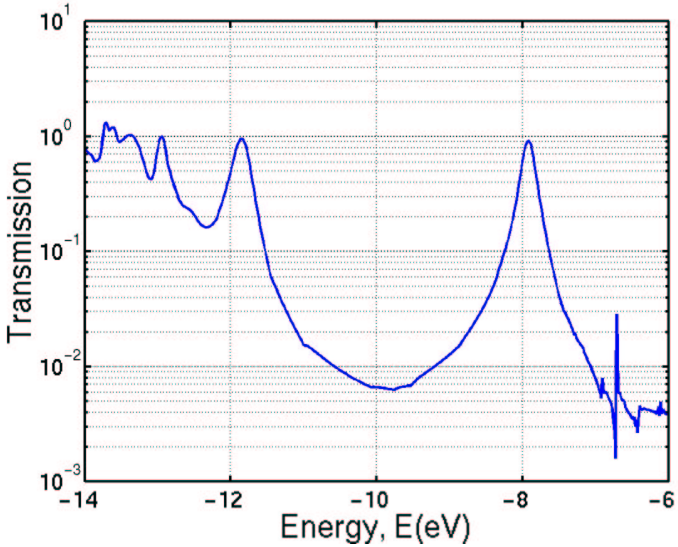
- [x] GIF (Graphic Interchange Format)
- [ ] PDF (Portable Document Format)
- [ ] PS (PostScript)

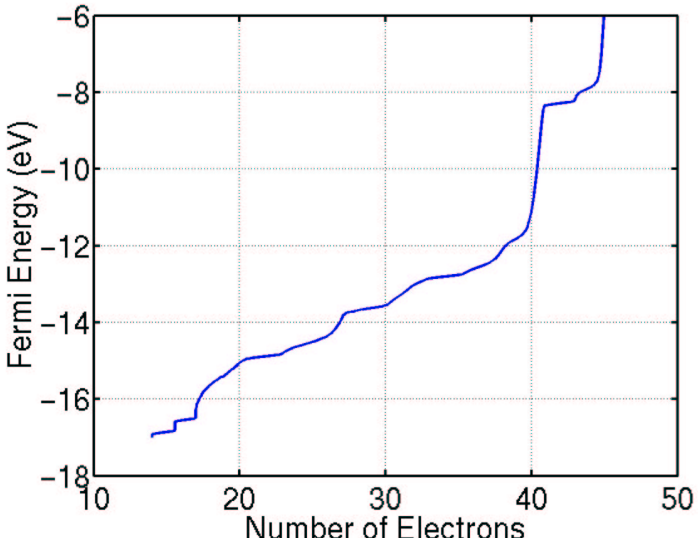
Output Folder: pdt

Calculate Properties

Exercise -2 : Output







E_c^{nl} = -1.08 eV

Exercise -3 : Procedure

- First upload the Dos_TE.mat file for PDT from the example folder in Output page (this file is already uploaded in the previous step)

- Next go to main Execute page and select 'Calculate Non-Equilibrium Properties (Non-Self-Consistent Method)'

- From 'Calculate Non-Equilibrium Properties (Non-Self-Consistent Method)' page select the Dos_TE.mat file and then put all other parameter values on the blank space correctly (parameter values can be obtained from the README file in example folder of Input page) and push **Calculate Properties** button

- In the 'Program Status' page keep pushing **Proceed** button until it says ' No Programs Executing'. It will take 1 to 3 minutes to finish.

- Then follow the same procedure from the 'Calculate Non-Equilibrium Properties (Self-Consistent Method)' page to do the self-consistent calculation

- Then go to the Output page and view gv_eta.gif and gv_scf.gif files

Exercise -3 : Procedure

Calculate Non-Equilibrium Properties (Non-Self-Consistent Method)

DOS and Transmission Data File: Dos_TE.mat
(from prior step)

Equilibrium Fermi Level, E_f: -11.0

Voltage Division Factor: 0.5

Voltage Grid

V min: -4

V max: 4

Bias Points, NV: 20

Plot Format(s) *(if any)*

- [x] GIF (Graphic Interchange Format)
- [ ] PDF (Portable Document Format)
- [ ] PS (PostScript)

Output Folder: pdt

Calculate Properties

Exercise -3 : Procedure

Calculate Non-Equilibrium Properties (Self-Consistent Method)

DOS and Transmission Data File: Dos_TE.mat
(from prior step)

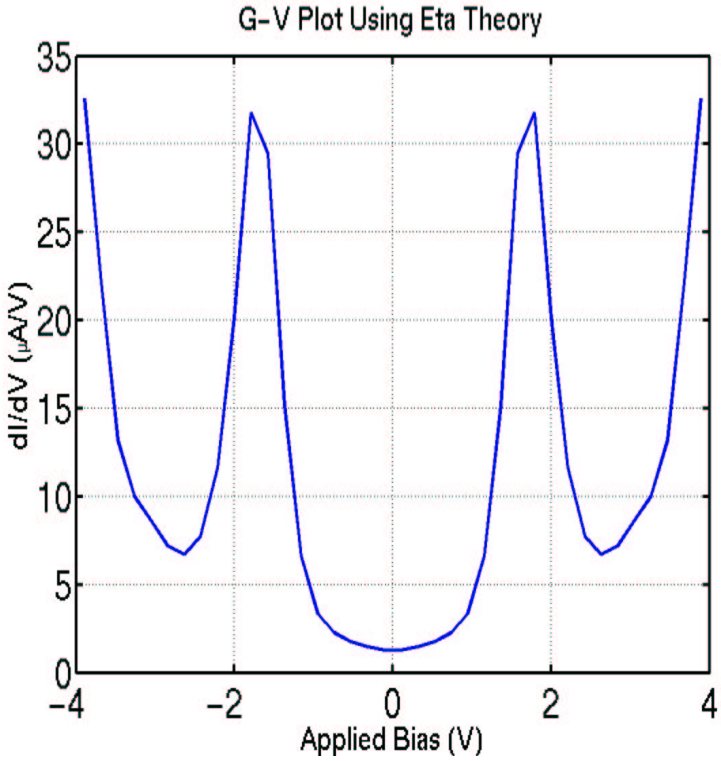
- Equilibrium Fermi Level, E_f: -11.0
- Charging Energy, U_0: 2.0
- Number of Electrons, N_eq: 40
- Voltage Grid
  - V min: -4
  - V max: 4
  - Bias Points, NV: 20
- Convergence Parameters
  - Number of Iterations: 200
  - Convergence Factor: 1e-3
  - Damping: 0.05

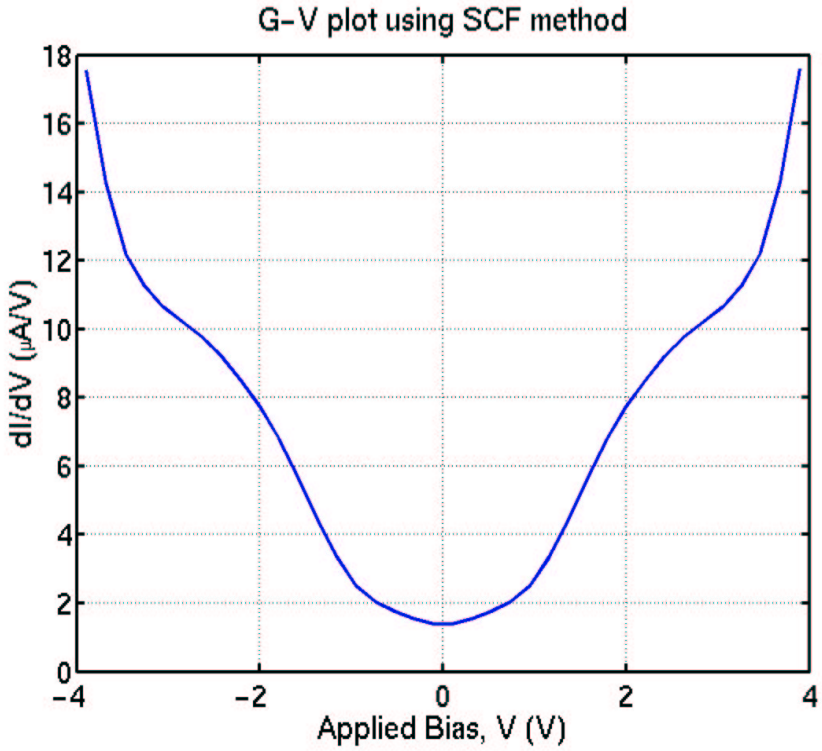
Plot Format(s) *(if any)*

- [x] GIF (Graphic Interchange Format)
- [ ] PDF (Portable Document Format)
- [ ] PS (PostScript)

Output Folder: pdt

Exercise -3 : Output





Exercise -4 : Procedure

- First upload the Dos_TE.mat file for PDT for asymmetric coupling from the example folder in Output page (this file is already created using Left Coupling Factor = 1 and Right Coupling Factor = 0.6). Copy the file from pdt_asym directory.

- Next go to main Execute page and select 'Calculate Non-Equilibrium Properties (Self-Consistent Method)'

- From 'Calculate Non-Equilibrium Properties (Self-Consistent Method)' page select the Dos_TE.mat file and then put all other parameter values on the blank space correctly (parameter values can be obtained from the README file in example folder of Input page) and push **Calculate Properties** button

- In the 'Program Status' page keep pushing **Proceed** button until it says ' No Programs Executing'. It will take 1 to 3 minutes to finish.

- Then go to the Output page and view gv_scf.gif file

Exercise -4 : Procedure

Calculate Non-Equilibrium Properties (Self-Consistent Method)

DOS and Transmission Data File: Dos_TE.mat
(from prior step)

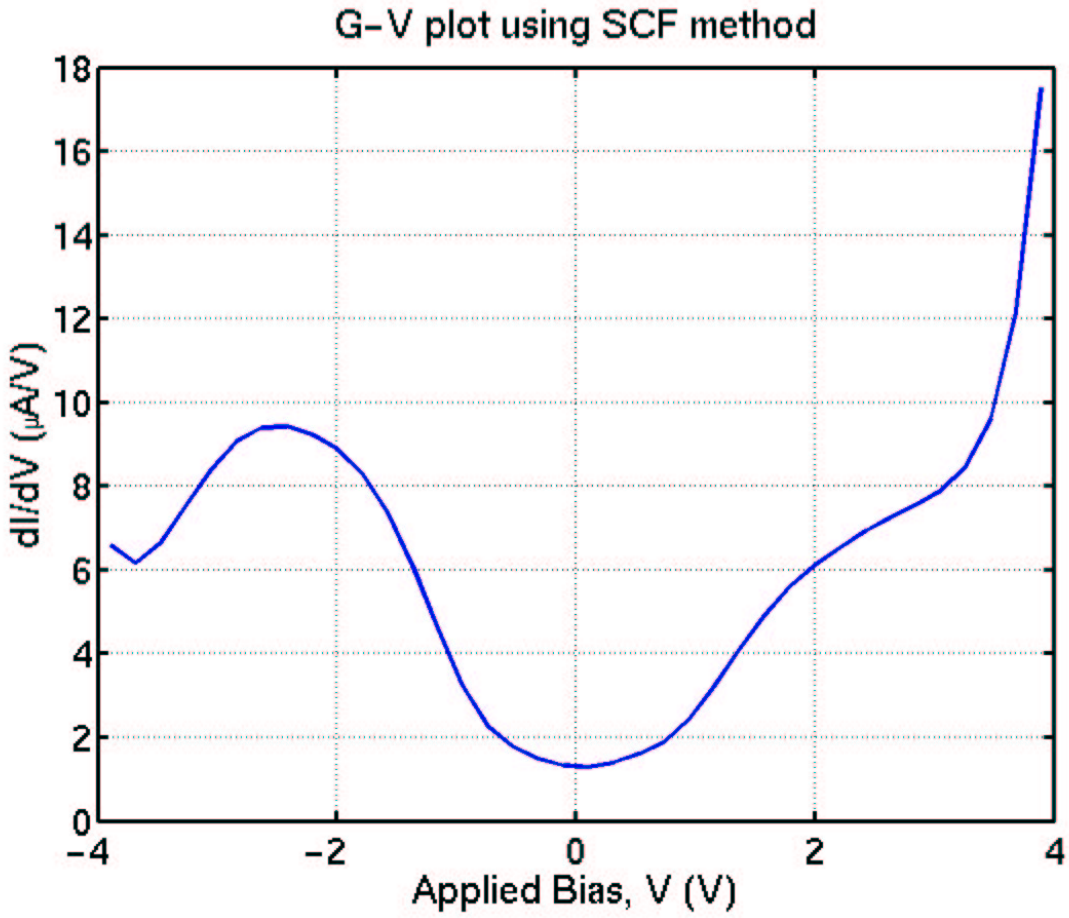
- Equilibrium Fermi Level, E_f: -10.5
- Charging Energy, U_0: 2.0
- Number of Electrons, N_eq: 40
- Voltage Grid
  - V min: -4
  - V max: 4
  - Bias Points, NV: 20
- Convergence Parameters
  - Number of Iterations: 200
  - Convergence Factor: 1e-3
  - Damping: 0.05

Plot Format(s) *(if any)*

- [x] GIF (Graphic Interchange Format)
- [ ] PDF (Portable Document Format)
- [ ] PS (PostScript)

Output Folder: pdt_asym

Exercise -4 : Output



Exercise -5 : Procedure

- First upload the Dos_TE.mat file for QPC from the example folder in Output page (copy the file from qpc directory)

- Next go to main Execute page and select ‘Calculate Non-Equilibrium Properties (Self-Consistent Method)’

- From ‘Calculate Non-Equilibrium Properties (Self-Consistent Method)’ page select the Dos_TE.mat file and then put all other parameter values on the blank space correctly (parameter values can be obtained from the README file in example folder of Input page) and push **Calculate Properties** button

- In the ‘Program Status’ page keep pushing **Proceed** button until it says ‘ No Programs Executing’. It will take 1 to 3 minutes to finish.

- Then go to the Output page and view iv_scf.gif file

Exercise -5 : Procedure

Calculate Non-Equilibrium Properties (Self-Consistent Method)

DOS and Transmission Data File: Dos_TE.mat
(from prior step)

- Equilibrium Fermi Level, E_f: -10.5
- Charging Energy, U_0: 2.0
- Number of Electrons, N_eq: 66
- Voltage Grid
  - V min: -1
  - V max: 1
  - Bias Points, NV: 20
- Convergence Parameters
  - Number of Iterations: 200
  - Convergence Factor: 1e-3
  - Damping: 0.05

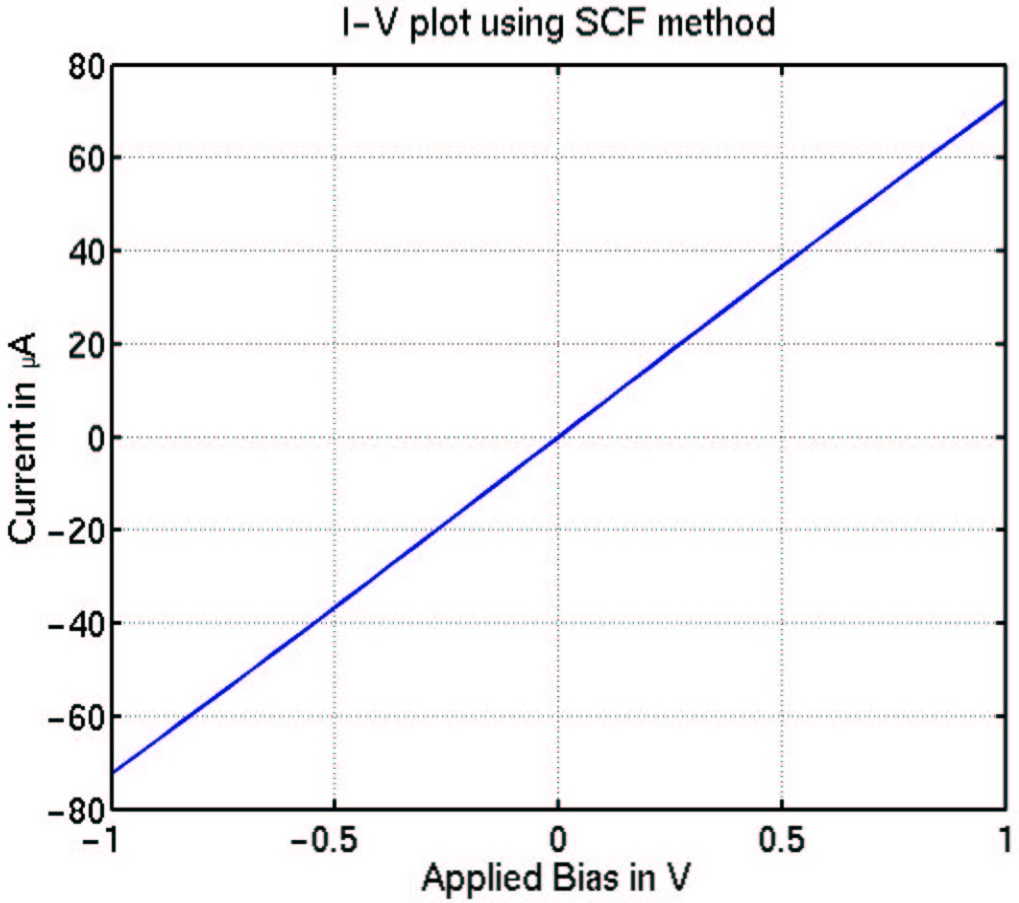
Plot Format(s) *(if any)*

- ☐ GIF (Graphic Interchange Format)
- ☐ PDF (Portable Document Format)
- ☐ PS (PostScript)

Output Folder: qpc

Calculate Properties

Exercise -5 : Output



The quantized conductance is around 75 μA/V

Exercise - Extra

Huckel-IV: Execute

Hub Directory | Huckel-IV | Step1:Input | Step2:Execute | Step3:Output

Help for *Step2:Execute* | **User:** molecule

Build Density of States (DOS) and Transmission Data Files

Coordinate File:	pdt_2H.dat	
	Left	Right
Position of End Atoms:	1	12
Pad Distance:	1.905	1.905
Coupling Factor:	1	1
Output Folder:	pdt	

Build DOS and Transmission Data

Few words on Huckel-IV codes

- All the codes of Huckel-IV are MATLAB codes except one
- Huckel.c is a C code which calculates the Hamiltonian and Overlap matrices using EHT
- Source codes of Huckel-IV can be downloaded from the main page of Huckel-IV on the hub
- All codes are documented and easy to understand