

2025 제 6회 전자구조계산 여름학교



Lab Session: 환경 설정 및 패키지 설치

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1. Linux 환경 만들기

a. Edison 웹 페이지

- <https://nano2.edison.re.kr/>
- JupyterLab terminal

b. Etc

- Server, linux, WSL

2. 패키지 설치

a. Atom

b. Siesta

c. QE

- Version 7.4
- Version 7.3 + patch



Edison 웹 페이지: <https://nano2.edison.re.kr/>

1. 계정 만들기



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New Customizable web-based first-principles* simulation designer

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for **Semiconductor Device Physics**

반도체 소자 물리 연구를 위한 손쉬운 R&D 플랫폼 - 직관적인 웹 기반 시뮬레이션 도구로 다양한 시나리오를 쉽게 테스트하고, 연구 개발을 더욱 빠르고 효율적으로 진행하세요.

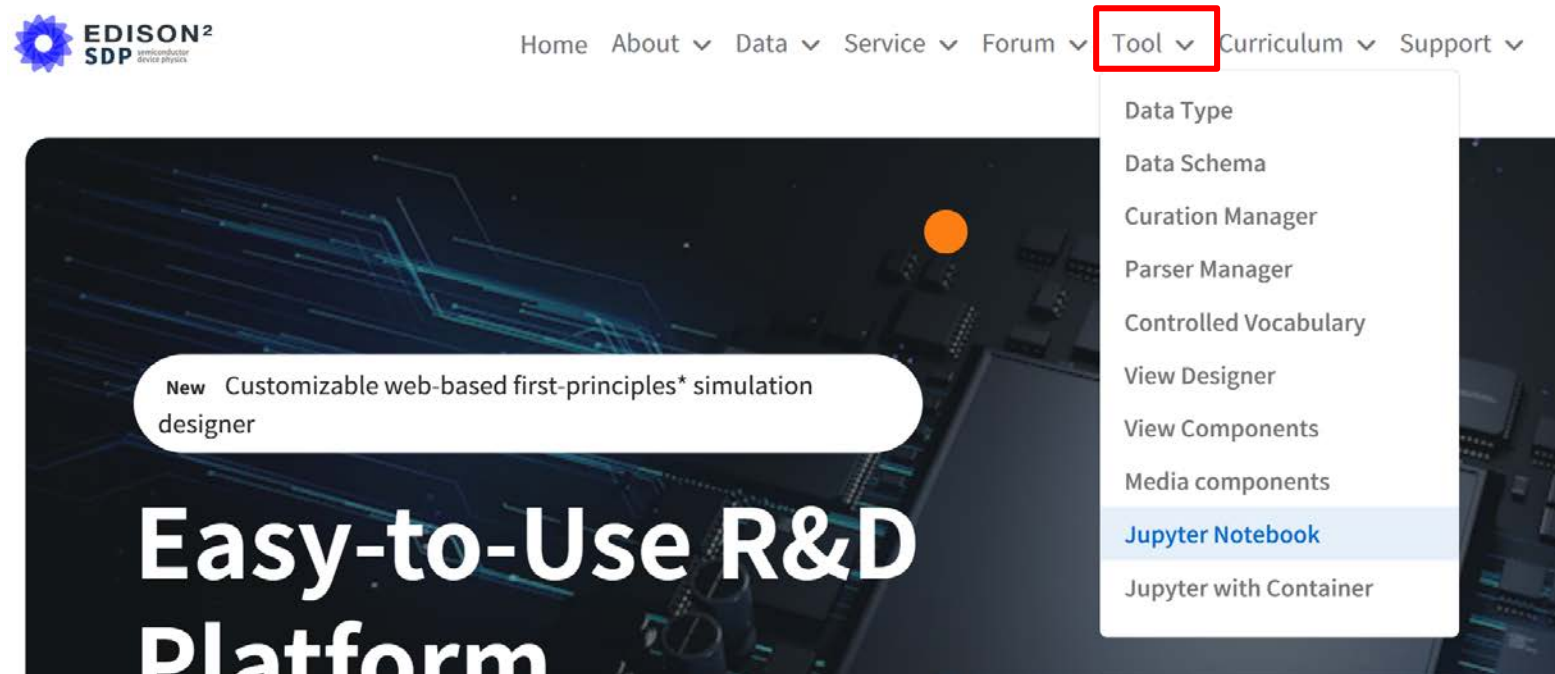


1-1 환경 설정 - Edison/JupyterLab

Edison 웹 페이지: <https://nano2.edison.re.kr/>

2. JupyterLab 열기

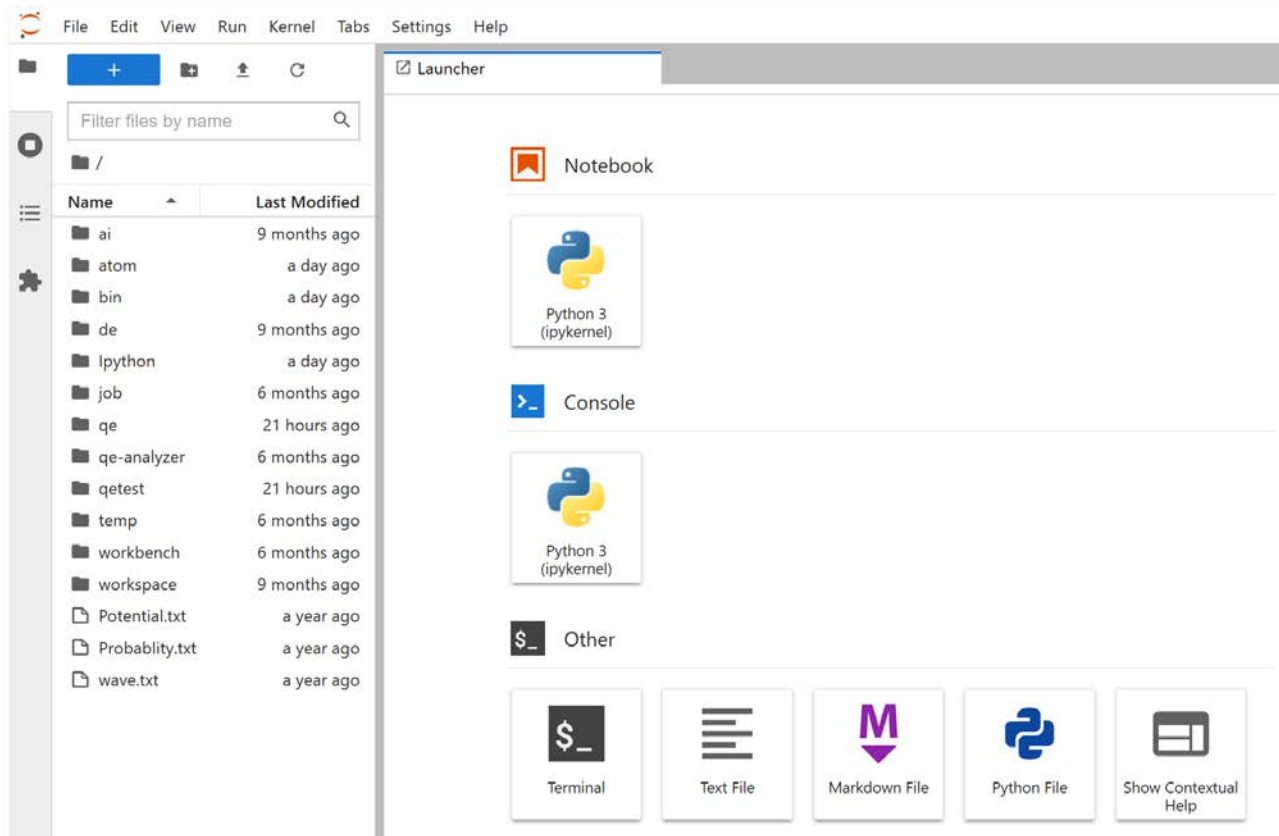
- Menu: Tool/Jupyter Notebook





3. JupyterLab 실습

- JupyterLab: Menu, File browser, Workspace
- Menu: File/New or [+] icon 클릭 → New tab
- Workspace: Tab으로 notebook, terminal 등이 열림
- File browser: .txt, .ipynb, .csv, .png (그림파일) 등은 바로 열림



4. Terminal

- Linux 사용

- https://yhkimlab.github.io/YHKimLabWiki/site/other/1.1_LinuxCheatSheet/

The screenshot displays the JupyterLab interface. On the left is a file browser showing a directory structure with files like `ae.gplot`, `ae.gps`, `ae.mkpng`, `ae.png`, `ae.ps`, `AECHARGE`, `AEWFNR0`, `AEWFNR1`, `CHARGE`, `charge.gplot`, `charge.gps`, `INP`, `INP_COPY`, and `OUT`. The main area contains a terminal window with the following commands and output:

```
hopeful@jupyter-hopeful:~$ source .bashrc
hopeful@jupyter-hopeful:~$ ls
ai  bin  lpython  Potential.txt  qe          qetest  wave.txt  workspace
atom  de  job  Probability.txt  qe-analyzer  temp    workbench
hopeful@jupyter-hopeful:~$ pwd
/home/hopeful
hopeful@jupyter-hopeful:~$ cd atom
hopeful@jupyter-hopeful:~/atom$ ls
atom-4.2.7-100  atom-4.2.7-100.tgz  libgridxc-0.8.5  libgridxc-0.8.5.tgz  xmlf90-1.5.0  xmlf90-1.5.0.tgz
hopeful@jupyter-hopeful:~/atom$ which conda
/opt/conda/bin/conda
hopeful@jupyter-hopeful:~/atom$ which pip
/opt/conda/bin/pip
hopeful@jupyter-hopeful:~/atom$ which gnuplot
/usr/bin/gnuplot
hopeful@jupyter-hopeful:~/atom$ pip install matplotlib
Collecting matplotlib
  Downloading matplotlib-3.9.4-cp39-cp39-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (8.3 MB)
    |████████████████████| 8.3 MB 7.7 MB/s
Collecting kiwisolver>=1.3.1
  Downloading kiwisolver-1.4.7-cp39-cp39-manylinux_2_12_x86_64.manylinux2010_x86_64.whl (1.6 MB)
    |████████████████████| 1.6 MB 40.7 MB/s
Collecting pillow>=8
  Downloading pillow-11.3.0-cp39-cp39-manylinux_2_27_x86_64.manylinux_2_28_x86_64.whl (6.6 MB)
    |████████████████████| 6.6 MB 30.2 MB/s
Requirement already satisfied: importlib-resources>=3.2.0 in /opt/conda/lib/python3.9/site-packages (from matplotlib) (5.4.0)
```

5. Jupyter notebook

- Encode python script
- 모듈 설치는 터미널에서 pip을 이용

The screenshot displays the JupyterLab environment. On the left, the file browser shows a directory structure with files like `ae.gplot`, `ae.gps`, `ae.mkpng`, `ae.png`, `ae.ps`, `AECHARGE`, `AEWFNR0`, and `AEWFNR1`. The main area contains a code editor with a single cell containing the following code:

```
[1]: import matplotlib
```

Below the code cell, a red error message is displayed, indicating a `ModuleNotFoundError` for the `matplotlib` module. The error message includes a traceback showing the location of the error and the specific error type.

```
-----  
ModuleNotFoundError                                Traceback (most recent call last)  
/tmp/ipykernel_169/1365702724.py in <module>  
----> 1 import matplotlib  
  
ModuleNotFoundError: No module named 'matplotlib'
```



5. png file

- Terminal에서 작업 후 png 파일 생성시 가시화

The screenshot displays the JupyterLab interface. On the left, the file explorer shows a directory structure with files like `ae.gplot`, `ae.gps`, `ae.mkpng`, `ae.png` (highlighted), `ae.ps`, `AECHARGE`, `AEWFNR0`, `AEWFNR1`, `CHARGE`, `charge.gplot`, `charge.gps`, `INP`, and `INP_COPY`. The main area contains two terminal windows and a plot window. The plot window shows two side-by-side plots. The left plot, titled 'AE wfn s', shows a purple curve with a minimum at x=0.5 and a maximum at x=1.5. The right plot, titled 'AE wfn p', shows a purple curve with a minimum at x=0.5 and a maximum at x=2.5.

Name	Last Modified
ae.gplot	a day ago
ae.gps	a day ago
ae.mkpng	an hour ago
ae.png	an hour ago
ae.ps	an hour ago
AECHARGE	a day ago
AEWFNR0	a day ago
AEWFNR1	a day ago
CHARGE	a day ago
charge.gplot	a day ago
charge.gps	a day ago
INP	a day ago
INP_COPY	a day ago

6. 자료 download

- git clone https://github.com/yhkimlab/ESC_School.git
- 매뉴얼 찾아 오른쪽 마우스로 Download
- source batch.sh
 - Text 파일 → double click으로 열기 → 수정

7. 파일 upload

- Icon 이용 파일 upload

The screenshot displays the JupyterLab interface. On the left, the file browser shows a list of files and folders. The 'SummerSchool6' folder, created 11 minutes ago, is highlighted with a red box. Above the file browser, the 'Run' button (represented by an upward arrow icon) is also highlighted with a red box. The main terminal window shows the execution of several commands:

```
hopeful@jupyter-hopeful:~ $ echo $SHELL
/bin/bash
hopeful@jupyter-hopeful:~ $ which git
/usr/bin/git
hopeful@jupyter-hopeful:~ $ git clone https://github.com/hopeful/SummerSchool6.git
Cloning into 'SummerSchool6'...
remote: Enumerating objects: 3, done.
remote: Counting objects: 100% (3/3), done.
remote: Compressing objects: 100% (3/3), done.
remote: Total 3 (delta 0), reused 0 (delta 0), pack-reused 0 (from 0)
Unpacking objects: 100% (3/3), 2.61 MiB | 5.59 MiB/s, done.
hopeful@jupyter-hopeful:~ $ ls
ai      batch.sh  de      job      Probablity.txt  qe-analyzer  SummerSchool6  wave.txt  workspace
atom    bin       Ipython Potential.txt  qe            qetest       temp           workbench
```

The terminal output continues with the user navigating into the 'SummerSchool6' directory and listing its contents, which include 'batch.sh' and 'workbench'.

1. Github

- a. <https://yhkimlab.github.io/YHKimLabWiki/site/>

2. Gnuplot 파일 수정

- a. ps 파일 대신에 png 파일로 쓰기
 - postscript
 - set terminal postscript enhanced color
 - set output "ae.ps"
 - png
 - set terminal pngcairo size 800,800 enhanced font 'Arial,12'
 - set output "ae.png"

1. 아나콘다 안에서 설치

- a. https://ytkimlab.github.io/YHKimLabWiki/site/build/build_siesta_local/#3-2-anaconda
- b. `conda install -c conda-forge siesta`
 - `/opt/conda/bin` 에 설치

2. 테스트

- a. Download
 - `siesta RUN.fdf`

Linux에 설치

```
bash batch.sh
```

Test

```
cd install/exercise_shin/lecture1/1.scf  
bash run.sh
```

batch.sh

```
mkdir install  
cd install  
wget https://gitlab.com/QEF/q-e/-/archive/qe-7.4/q-e-qe-7.4.tar  
tar -xvf q-e-qe-7.4.tar  
cd q-e-qe-7.4  
./configure  
make pw pp
```

Linux에 설치 순서

Modify make.inc

1. bash batch1.sh
2. Modify make.inc
3. bash batch2.sh

FFLAGS 및 FFLAGS_NOOPT 줄 끝에
"-ffree-line-length-none"을 추가

Batch 2

make depend
make pw pp

Batch 1

```
git clone -b qe-7.3 https://gitlab.com/QEF/q-e.git  
git clone https://github.com/KIAS-CMT/DFT-U-V.git  
cd DFT-U-V  
cp qe-7.3_ehub_uv.diff ../q-e/  
cd ../q-e  
./configure  
patch -p1 < qe-7.3_ehub_uv.diff
```