To run the script on a **fresh Windows installation** without any prior software, you'll need to install the following dependencies:

**1. Install Required Software**

**A. Python Environment**

1. **Download & Install Python 3.x** (latest stable version)
   * **Get it from:** <https://www.python.org/downloads/>
   * Make sure to check **"Add Python to PATH"** during installation.
2. **Install Pip (Package Manager)** (Usually comes with Python, but verify)
   * Open **Command Prompt** and run:

sh

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python -m ensurepip --default-pip

**B. Quantum ESPRESSO (QE)**

1. **Download & Install Quantum ESPRESSO for Windows**
   * **Get it from:** https://www.quantum-espresso.org/download/
   * Ensure pw.exe, bands.exe, and dos.exe are available in the qe directory.
2. **Install Microsoft MPI (Message Passing Interface)**
   * **Get it from:** <https://www.microsoft.com/en-us/download/details.aspx?id=57467>
   * Required for mpiexec -np X commands.

**2. Install Python Dependencies**

After installing Python, open **Command Prompt** and run:

sh

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pip install numpy matplotlib pymatgen mp-api scipy curses openai

This installs:

* numpy – for numerical computations.
* matplotlib – for plotting band structures & DOS.
* pymatgen – for retrieving material data & generating QE input files.
* mp-api – to interact with the Materials Project API.
* scipy – for signal processing.
* curses – for text-based UI (Windows may require windows-curses instead).
* openai – for AI\_perp.py to use the Perplexity API.

**For Windows**, you may need to install windows-curses:

sh

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pip install windows-curses

**3. External API Keys Needed**

1. **Materials Project API Key** – Required for generate\_qe\_inputs.py
   * Store in api\_keys/api\_key\_mp.txt
   * Get it from [Materials Project](https://materialsproject.org/)
2. **Perplexity API Key** – Required for AI\_perp.py
   * Store in api\_key\_perp.txt
   * Get it from [Perplexity AI](https://www.perplexity.ai/)

**4. Folder & File Setup**

Ensure your project directory looks like this:

graphql

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/YourProject/

│-- qe/ # Quantum ESPRESSO binaries

│-- api\_keys/

│ ├── api\_key\_mp.txt # Materials Project API Key

│ ├── api\_key\_perp.txt # Perplexity API Key

│-- python\_dependencies/

│ ├── welcome.py

│ ├── generate\_qe\_inputs.py

│ ├── plot\_bands.py

│ ├── plot\_dos.py

│ ├── AI\_perp.py

│-- inputs/ # QE input files will be stored here

│-- outputs/ # QE output files will be stored here

│-- pseudo/ # Pseudopotentials

│-- tmp/ # Temporary files

│-- run\_calculator.bat # The batch script you posted

**5. Running the Script**

Once everything is installed, navigate to your project folder and double-click run\_calculator.bat, or run:

sh

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cd path\to\YourProject

run\_calculator.bat

This should initialize the **Neuromorphic Calculator 2.0** workflow.

**Final Checklist**

✅ Install **Python 3.x**  
✅ Install **Quantum ESPRESSO & MPI**  
✅ Install **Required Python packages**  
✅ Setup **API keys for MP & Perplexity**  
✅ Organize **folders & scripts correctly**  
✅ Run run\_calculator.bat