



Quantum Espresso is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

I have already shown you how to download, install and run Quantum Espresso on Linux [here](#).

In this post I will do the same for Windows.

DOWNLOAD:

In my limited knowledge I noticed that the latest version of Quantum Espresso, that is version 6.1, isn't available for windows. As one can check here:

http://qe-forge.org/gf/project/q-e/frs/?action=FrsReleaseBrowse&frs_package_id=18

The latest version available for Windows is 5.3.

You can download it from [here](#).

The binaries available for both 32 and 64-bit versions. You can download them according to your pc configurations. It should also be noted that QE on windows uses mpich for parallel processing.

INSTALLATION:

Once downloaded, the installation procedure is really simple. Just double click on the installer(setup) and follow the instructions.

DEMO:

If you successfully installed QE then, you can run a simple demo now to see if the things work as they should. Let's perform an SCF calculation for Silicon for demo purpose.

To perform such a calculation, you need an input file for Quantum Espresso. You can download the sample input file from this link([si.scf](#)). Once you have the file, save it in a folder of your choice. For the sake of this tutorial, let's say you save it in a folder called 'QE' inside the Quantum Espresso installation directory.

Now, create a folder called 'temp' inside the directory that contains the input file(in our example the folder is 'QE').

Now let me tell you a little about the input file that we have here. In this file, we are basically trying to find out some of the properties for a Si atom, like the total energy, etc.

The input file is a really important file and you will need to learn quite a few things to be able to build one yourself. There are a lot of things that need explaining there, but I guess I will leave that for another post, and in this tutorial we will, just focus on running our first pw scf calculation. For the sake of the tutorial you can download the input file that I will be using from here([Si_Quantum_Espresso_input](#)) or you can just copy the following and save it in a file called `si.scf.in`.

```
&CONTROL
calculation = "scf"
max_seconds = 8.64000e+04
pseudo_dir = "F:/QE/"
outdir="temp"
/

&SYSTEM
a = 5.46873e+00
degauss = 1.00000e-02
ecutrho = 1.00000e+02
ecutwfc = 2.50000e+01
ibrav = 1
nat = 8
ntyp = 1
occupations = "smearing"
smearing = "gaussian"
/

&ELECTRONS
conv_thr = 1.00000e-06
electron_maxstep = 200
mixing_beta = 7.00000e-01
startingpot = "atomic"
startingwfc = "atomic+random"
/

K_POINTS {automatic}
2 2 2 0 0 0

ATOMIC_SPECIES
Si 28.08550 Si.pbe-rrkj.UPF

ATOMIC_POSITIONS {angstrom}
Si 0.000000 0.000000 0.000000
Si 4.101546 4.101546 1.367182
Si 0.000000 2.734364 2.734364
Si 4.101546 1.367182 4.101546
Si 2.734364 0.000000 2.734364
Si 1.367182 4.101546 4.101546
Si 2.734364 2.734364 0.000000
Si 1.367182 1.367182 1.367182
```

Make sure you copy and paste the above code in a file called `si.scf.in`.

Now, you can run an scf calculation by using the following command in the command prompt:

```
pw <si.scf.in> si.scf.out
```

However, if you run the above command simply as it is, then it won't work.

There are a few things you should keep in mind before running the above command.

You need to get the pseudopotential for your atom.

If you open the input file using a text editor, you will notice the field: `pseudo_dir = ' '` inside the `&control` section.

Inside the single quotes you need to specify the directory of your pseudopotential. But before that you first need to download one from here. Once you go to the link you can click on any atom to get a list of its available pseudopotentials. For this tutorial, we need a particular potential for Si. So click on Si(14) in the periodic table shown. Now you will see a list of a variety of potentials. Just search for this one : `'Si.pbe-rrkj.UPF'` and download it.

Make sure you change the address to specify the folder containing the Pseudopotential.

Now, you should open Command Prompt, and change the directory to the one containing the above `si.scf.in` file.

Now, the command will work,

```
pw <si.scf.in> si.scf.out
```

Once the execution is complete, you will see a file called `si.scf.out` created in the same folder/directory.

You can open it using any text editor and read the values of total energy at each iteration and the Fermi Energy.

PROJECT FILES:

Zip File: [Si_Quantum_Espresso_input](#)

RESOURCES & REFERENCES:

Readers might find the following manual helpful:

<http://qe-forge.org/gf/download/frsrelease/204/922/QE-on-Windows.pdf>

More QE examples:

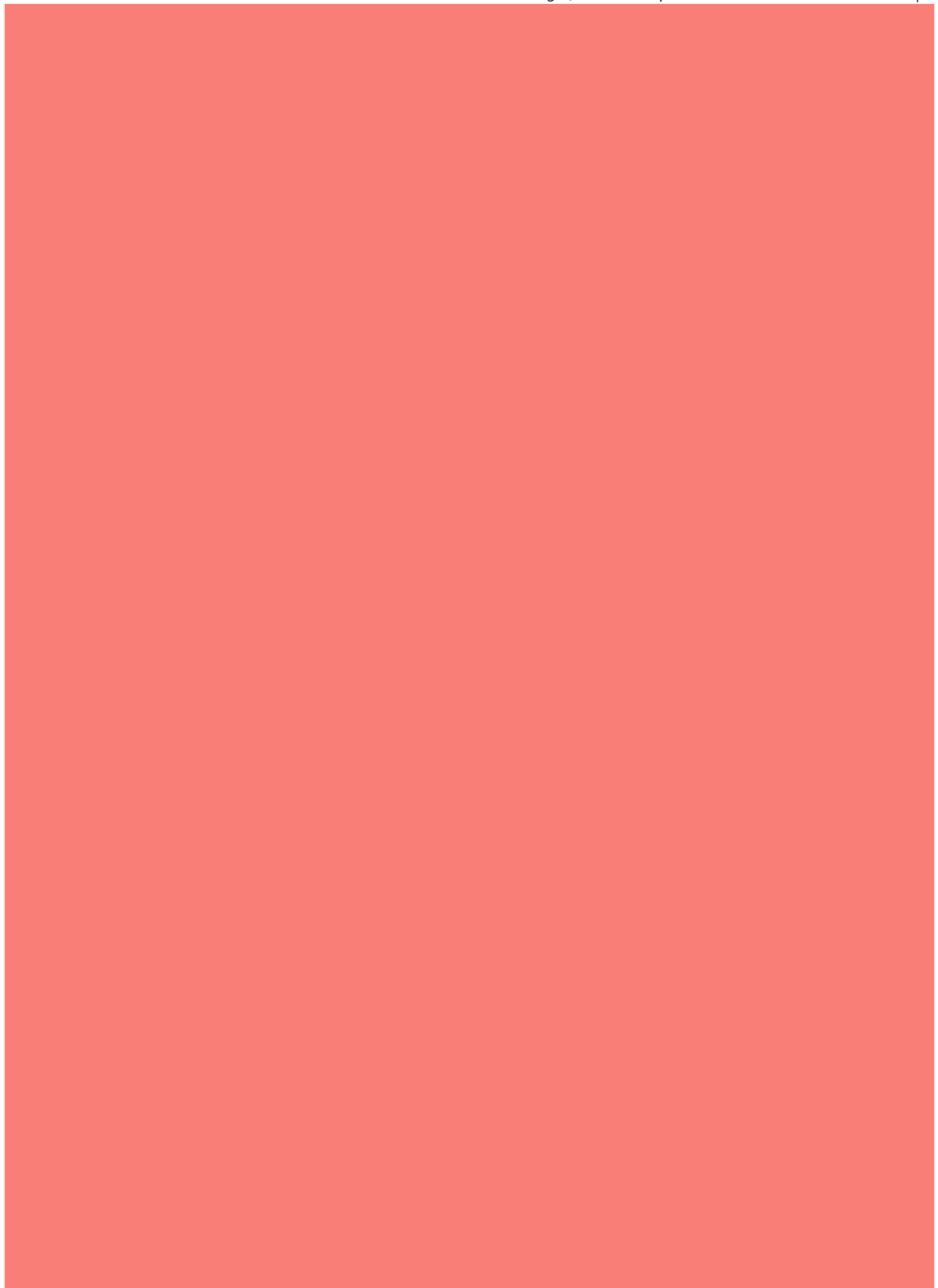
<http://qe-forge.org/gf/download/frsrelease/240/1072/qe-6.1-examples.tar.gz>

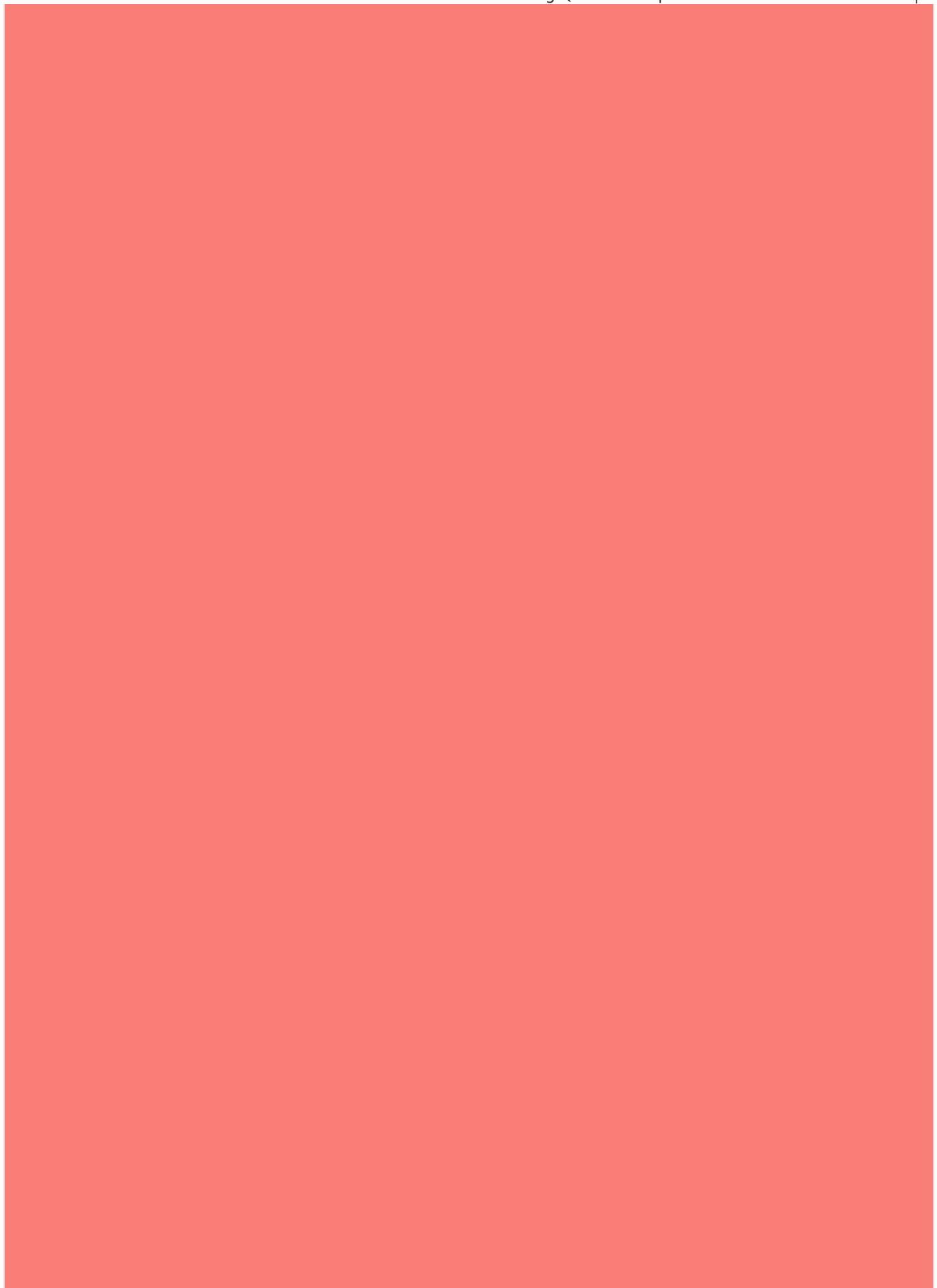


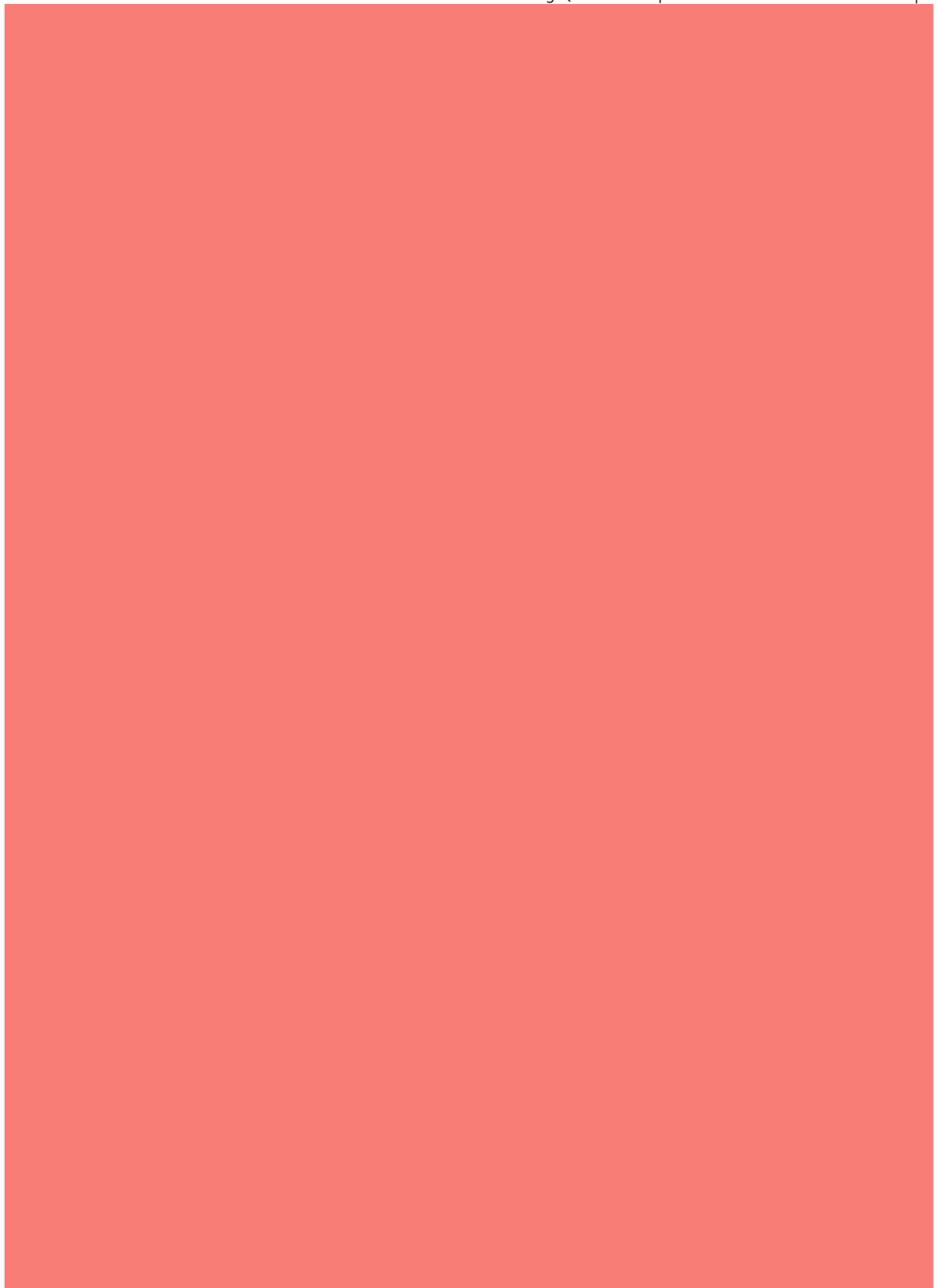
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I'm a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from time to time. Can code in most of the popular languages. I like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

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