TURBOMOLE is a widely used quantum chemistry software package for calculations on molecular systems. It offers a range of methods including Hartree-Fock, density functional theory, many-body perturbation theory, and coupled cluster. In this blog post, I'll walk through the steps to install TURBOMOLE and verify that it is working correctly.

Downloading and Unpacking

First, download the latest version of TURBOMOLE from the official website. It is distributed as a tar archive file.

After downloading, unpack the archive:

```
gunzip turbomole_XX.tar.gz
tar -xvf turbomole_XX.tar
```

This will extract the TURBOMOLE directory structure.

Note: Do not install or run TURBOMOLE as the root user! This can cause issues with permissions. Extract the files as a normal user.

Setting Environment Variables

Before using TURBOMOLE, some environment variables need to be set:

```
export TURBODIR=/path/to/turbomole # TURBOMOLE installation directory
source $TURBODIR/Config_turbo_env   # Sets paths correctly
```

The `Config_turbo_env` script will set up the `PATH` and other variables needed to run TURBOMOLE programs.

Testing the Installation

To verify that TURBOMOLE is installed correctly, run the test suite located in `$TURBODIR/TURBOTEST`:

```
cd $TURBODIR/TURBOTEST
TTEST
```

This will run a series of test calculations and check the results. All tests should pass if TURBOMOLE is properly installed.

If tests fail, it likely indicates limits on stack size or memory are too low. These need to be increased – please refer to the TURBOMOLE documentation for details.

Running a Sample Calculation

As a final test, we can perform a simple single-point DFT calculation.

First, create a file called `coord` that contains the atomic coordinates in bohrs (TURBOMOLE format), i.e. the following

```
$coord
   -0.72176422179068      -0.21015305295025      -0.00000000000017      o
   -0.04244721981318       1.49030097360157       0.00000000000008      h
    0.76421144160386      -1.28014792065131       0.00000000000008      h
$end
```

Then, create an input file named `control` with the following:

```
$atoms
  basis = def2-SVP
$coord file=coord
$dft
   functional pbe
$end
```

This input specifies a water molecule in a minimal basis set at the PBE/DFT level of theory.

Then run:

```
dscf > dscf.out
```

This will perform the calculation, writing output to `dscf.out`.

If the calculation completes successfully, TURBOMOLE is installed correctly and ready for production use!

Summary

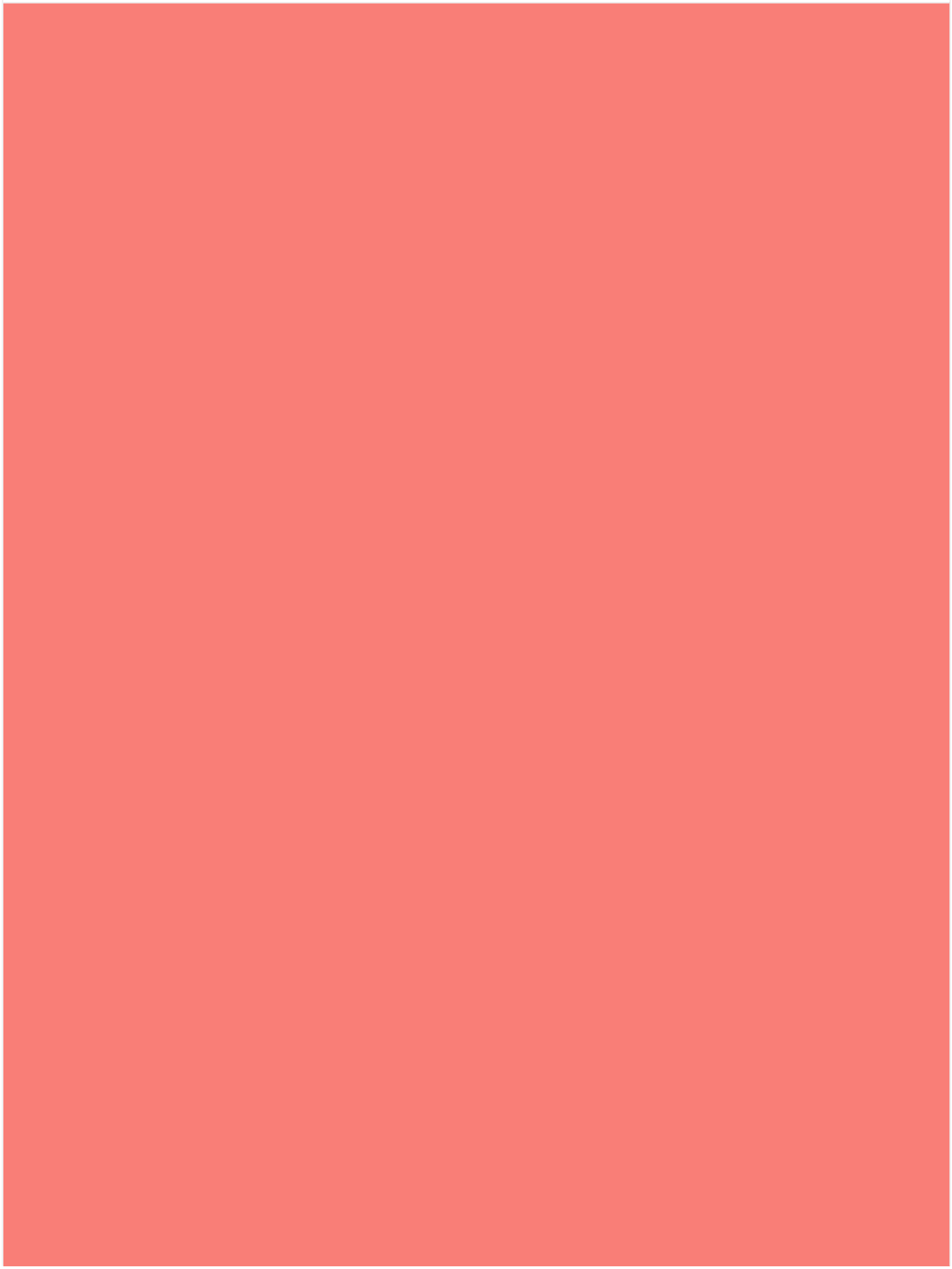
Installing TURBOMOLE involves unpacking the archive, setting environment variables, and running test calculations. By verifying the test suite passes and running a sample input, we can ensure TURBOMOLE is properly installed before tackling real projects. The documentation provides additional details on configuration and usage.

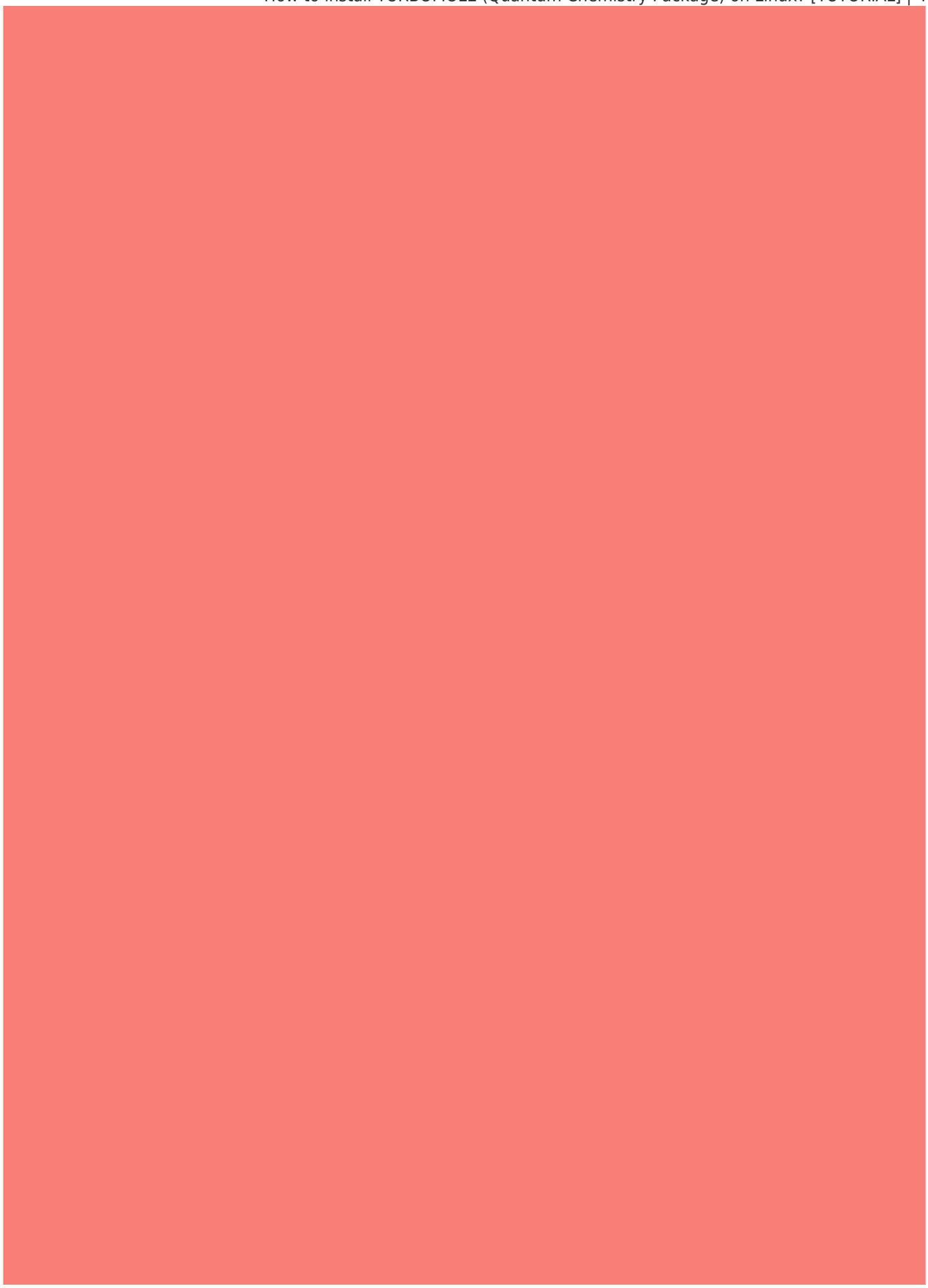
Please let me know if you still have any questions or doubts in the comments section down below.

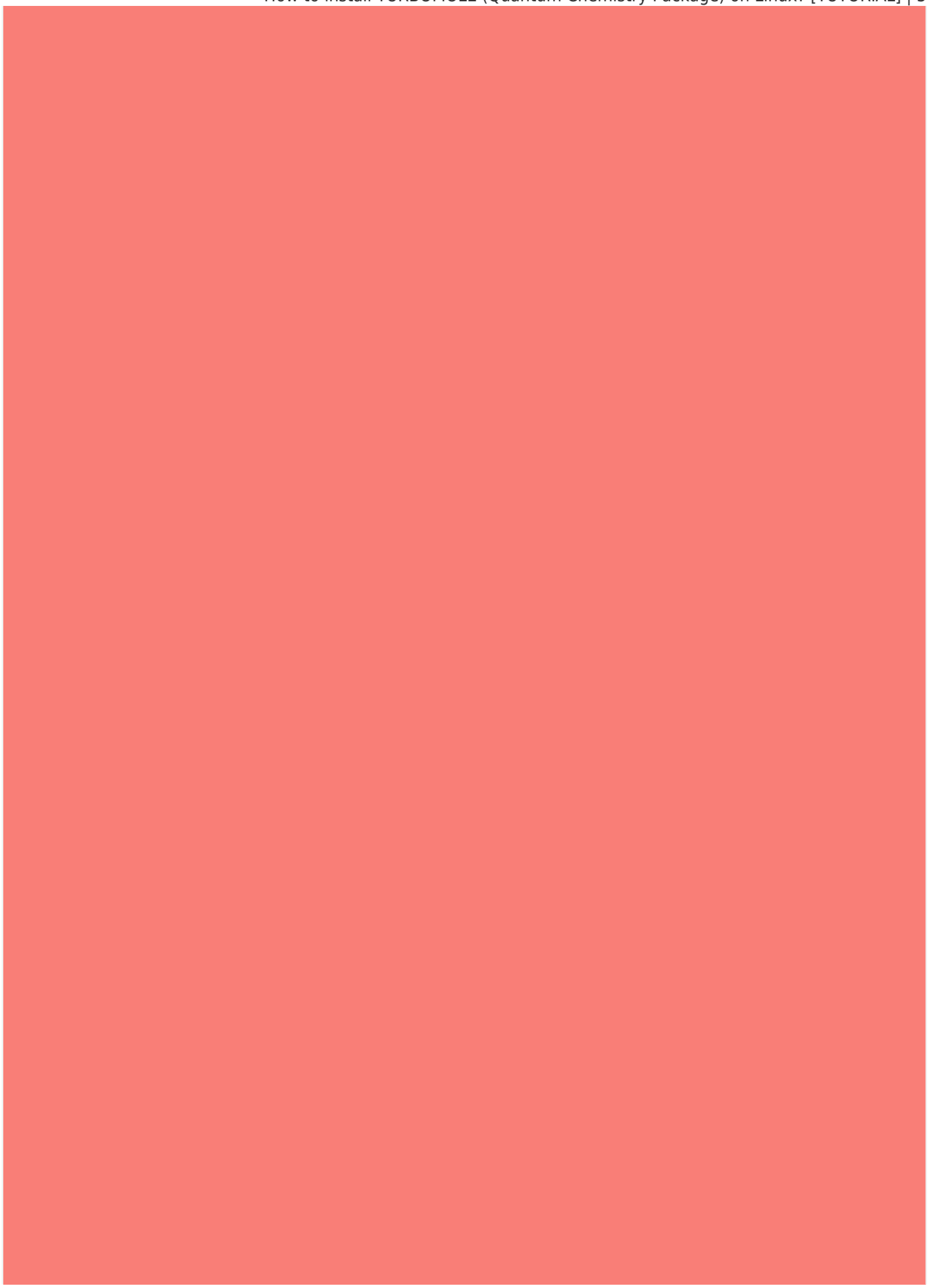


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I'm a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, 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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