

File Conversion from QE to YAMBO

In this tutorial we are going to learn how to convert QE generated wavefunctions into YAMBO readable format. We need *p2y*, and *yambo* executables to make this file conversion. For simplicity we copy these executables inside the “MoS2.save” directory (this is not standard practice, but it makes things easier to understand the first time).

```
$ cd MoS2.save
$ cp ../q-e-qe-6.4-rc/yambo-stable/bin/p2y ./
$ cp ../q-e-qe-6.4-rc/yambo-stable/bin/yambo./
```

At this point we have the executable *p2y* in the “MoS2.save” directory.

Now apply the following command to make the conversion,

```
$ ./p2y
```

At the end of the conversion you should see the flowing run-time output message if you have successfully converted the files,

```
.
.
.
.
<07s> == DB1 (Gvecs and more) ...
<07s> ... Database done
<07s> == DB2 (wavefunctions) ...
done ==
<01m-26s> == DB3 (PseudoPotential) ...
done ==
<02m-47s> == P2Y completed ==
```

At this step, you have successfully converted the QE generated wavefunctions into YAMBO readable format. Files are stored in a directory named; “SAVE” inside your “MoS2.save” directory.

Now apply the following command to initialize YAMBO and to test that everything runs well,

```
$ ./yambo
```

You should have the following run-time output at the end,

```
.  
.   
.   
.   
.   
E) 02s(X)  
<11s> SE indexes |#####| [100%] 02s  
(E) 02s(X)  
<16s> [04] Timing Overview  
<16s> [05] Game Over & Game summary
```

Finally, we have completed the conversion and the system should be ready for YAMBO calculations.