

# Quantum Espresso

## Singularity

q FeO\_test.in 723090ib pw.x

```
#BSUB -J FeO_test
#BSUB -q 723090ib
#BSUB -gpu num=1

module load singularity/latest

export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
SINGULARITY="singularity run --nv /fs00/software/singularity-images/ngc_quantum_espresso_qe-7.1.sif"
${SINGULARITY} pw.x < FeO_test.in > FeO_test.out
```

Revision #1

Created 17 November 2022 21:31:23 by LadderOperator

Updated 8 February 2023 23:08:01 by LadderOperator