

Quantum Espresso

??Apptainer

qe7.1

Fe0_test.in

1 GPU

723090ib

pw.x

```
#BSUB -J Fe0_test
#BSUB -q 723090ib
#BSUB -gpu num=1

export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
QE="apptainer run --nv /fs00/software/singularity-images/ngc_quantum_espresso_qe-7.1.sif"
${QE} pw.x < Fe0_test.in > Fe0_test.out
```

Revision #2

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