

	Step	FC	Time	Energy	fmax
*Force-consistent energies used in optimization.					
BFGSLineSearch:	0	[0]	11:01:52	5.911243*	1.0430
BFGSLineSearch:	1	[2]	11:01:52	5.581705*	1.1466
BFGSLineSearch:	2	[4]	11:01:52	5.506671*	0.3204
BFGSLineSearch:	3	[5]	11:01:53	5.499464*	0.1797
BFGSLineSearch:	4	[7]	11:01:53	5.465269*	0.8446
BFGSLineSearch:	5	[10]	11:01:53	5.439846*	0.8006
BFGSLineSearch:	6	[11]	11:01:53	5.383279*	0.3794
BFGSLineSearch:	7	[12]	11:01:53	5.366074*	0.2622
BFGSLineSearch:	8	[13]	11:01:53	5.353435*	0.3095
BFGSLineSearch:	9	[15]	11:01:53	5.345301*	0.1689
BFGSLineSearch:	10	[17]	11:01:53	5.337441*	0.1080

the Platinum energy before:
5.20297190996

```
#PBS -N job1
#PBS -q force
#PBS -o job1.output.$PBS_JOBID
#PBS -j oe
#PBS -l nodes=1:ppn=2
#PBS -l walltime=10:00

cd ./test.py/
source /nv/pace-ice/bcomer3/ug_esp_env.sh
python test.py
```