

```
$ ase build H2 | ase run nwchem -p xc=PBE -f .02
```

```
Running: H2
```

	Step	Time	Energy	fmax
LBFGS :	0	15:04:19	-31.487747	0.6220
LBFGS :	1	15:04:19	-31.492828	0.0378
LBFGS :	2	15:04:19	-31.492848	0.0020