```
>>> from ase import Atoms
>>> from ase.optimize import BFGS
>>> from ase.calculators.nwchem import NWChem
>>> from ase.io import write
>>> h2 = Atoms('H2',
...            positions=[[0, 0, 0],
...                       [0, 0, 0.7]])
...
>>> h2.calc = NWChem(xc='PBE')
>>> opt = BFGS(h2)
>>> opt.run(fmax=0.02)
BFGS:    0  19:10:49      -31.435229          2.2691
BFGS:    1  19:10:50      -31.490773          0.3740
BFGS:    2  19:10:50      -31.492791          0.0630
BFGS:    3  19:10:51      -31.492848          0.0023
>>> write('H2.xyz', h2)
>>> h2.get_potential_energy()
-31.492847800329216
```