#!/usr/bin/env python

from ase.calculators.vasp import Vasp

from ase import Atoms, Atom

from ase.io import read, write

atoms = read("POSCAR")

try:

with open("ncores") as f:

ncores = f.read().strip()

except FileNotFoundError:

ncores = "1"

calc = Vasp(

command=f"mpirun -np {ncores} /home/groups/gp-tej.choksi/vasp/vasp.6.4.2/bin/vasp\_std",

xc="pbe",

ivdw=11,

encut=400,

kpts=[11, 11, 11],

gamma=False,

ismear=1,

isym=2,

ibrion=2,

algo="Fast",

ediffg=-0.02,

ediff=1e-5,

lreal="Auto",

isif=3,

nsw=1000,

ispin=1, # 1: off 2: on

lcharg=False,

lwave=False,

)

atoms.calc = calc

e = atoms.get\_potential\_energy()

write("out.traj", atoms)

with open("final.e", "w") as f:

f.write(str(e) + "\n")

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