

AMD EPYC Rome

VASP

2019.11.18

Ruddlesden-Popper $\text{Sr}_4\text{Ti}_3\text{O}_{10}$ 305

```
SYSTEM = STO
```

```
PREC=A
```

```
ENCUT=520
```

```
EDIFF=1E-6
```

```
ADDGRID=.T.
```

```
ISMEAR= 1
```

```
SIGMA=0.2
```

```
LWAVE=.F.
```

```
LCHARG=.F.
```

```
NELMIN=4
```

```
NELM=100
```

```
LREAL=Auto
```


```
K-Points
```

```
0
```













Gamma

2 2 1

0 0 0

eScience 
10.1.243

VASP5.4.4 Intel 2018  CUDA

	CPU 	Elapsed time (s)	scf 	E0 in OSZICAR
e5v3ib  2*Intel Xeon E5-2680 v3 (12 Cores 2.50 GHz) 256 G RAM	24	6676	23	-.23554005E+04
e52682v4opa  , 2*Intel Xeon E5-2682 v4 (16 Cores, 2.50 GHz)	32	5967	23	-.23554005E+04
6140ib  , 4*Intel Xeon Gold 6140 (18 Cores, 2.30 GHz) 384 G RAM	72	2080	23	-.23554005E+04
6140ib  , 4*Intel Xeon Gold 6140 (18 Cores, 2.30 GHz) 384 G RAM	36	2456	23	-.23554005E+04
6140ib  , 4*Intel Xeon Gold 6140 (18 Cores, 2.30 GHz) 384 G RAM	18	5005	23	-.23554005E+04
7702  , 2*AMD EPYC 7702 (64 Cores, 256MB Cache, 2.0 GHz) 256 G RAM	32	5034	23	-.23554005E+04
7702  , 2*AMD EPYC 7702 (64 Cores, 256MB Cache, 2.0 GHz) 256 G RAM	64	3663	22	-.23554005E+04
7702  , 2*AMD EPYC 7702 (64 Cores, 256MB Cache, 2.0 GHz) 256 G RAM	128	4401	23	-.23554005E+04
7502  , 2*AMD EPYC 7502 (32 Cores, 128MB Cache, 2.5 GHz) 256 G RAM	32	5290	23	-.23554005E+04

节点	CPU/GPU	Elapsed time (s)	scf节点	E0 in OSZICAR
gpu_v100节点 8 X TESLA V100 NVLink GPU 2 X CPU intel Xeon Gold 6248, 20 核 2.5GHz, 768GB 内存	4/4	1379.651	23	-.23554005E+04
gpu_v100节点 8 X TESLA V100 NVLink GPU 2 X CPU intel Xeon Gold 6248, 20 核 2.5GHz, 768GB 内存	8/8	1214.461	23	-.23554005E+04



- AMD EPYC Rome 核 Intel V3/V4 节点 Intel Gold 节点
- 节点 VASP节点