

AMD EPYC Rome

VASP

 2019.11.18



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



```
SYSTEM = ST0
```

```
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 |

| □□□□ | CPU □□ | Elapsed time (s) | scf□□ | E0 in OSZICAR |
|---|-----------|------------------|-------|----------------|
| 7502□□ , 2*AMD EPYC 7502 (32 Cores, 128MB Cache, 2.5 GHz) 256 G RAM | 64 | 4176 | 22 | -.23554005E+04 |
| 62v100ib□□□□ 2*Intel Xeon Gold 6248 (20 Cores, 27.5MB Cache, 2.50 GHz) 768 GB RAM□ 8*NVIDIA Tesla V100 SXM2 32GB (5120 CUDA Cores 1290MHz, 32GB HBM2 876MHz 4096-bit 900 GB/s, NVLink, PCI-E 3.0 x16) | 1CPU 1GPU | 3053 | 23 | -.23554005E+04 |



VASP 5.4.4 Intel 2017□ CUDA

10.1.168

| □□□□ | CPU/GPU | Elapsed time (s) | scf□□ | E0 in OSZICAR |
|---|---------|------------------|-------|----------------|
| fat_384□□□ 4*Intel Xeon Gold 6248 (20 Cores, 2.50 GHz) 384 G RAM | 20 | 5326.949 | 23 | -.23554005E+04 |
| fat_384□□□ 4*Intel Xeon Gold 6248 (20 Cores, 2.50 GHz) 384 G RAM | 40 | 3105.863 | 23 | -.23554005E+04 |
| fat_384□□□ 4*Intel Xeon Gold 6248 (20 Cores, 2.50 GHz) 384 G RAM | 80 | 2896.237 | 21 | -.23554005E+04 |
| gpu_v100□□□ 8 X TESLA V100 NVLink GPU□ 2 X CPU intel Xeon Gold 6248, 20 □□ 2.5GHz, 768GB □□ | 1/1 | 3202.687 | 23 | -.23554005E+04 |
| gpu_v100□□□ 8 X TESLA V100 NVLink GPU□ 2 X CPU intel Xeon Gold 6248, 20 □□ 2.5GHz, 768GB □□ | 2/2 | 2244.153 | 23 | -.23554005E+04 |

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



- AMD EPYC Rome □ Intel V3/V4 □□□□□ Intel Gold □□□□
- □□□□□ VASP□□□□

Revision #6

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