

AMD EPYC Rome VASP

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2019.11.18

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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
```

eScience????????VASP5.4.4 Intel 2018?CUDA 10.1.243

配置	CPU 核数	Elapsed time (s)	scf步数	E0 in OSZICAR
e5v3ib配置, 2*Intel Xeon E5-2680 v3 (12 Cores 2.50 GHz) 256 G RAM	24	6676	23	-.23554005E+04
e52682v4opa配置, 2*Intel Xeon E5-2682 v4 (16 Cores, 2.50 GHz)	32	5967	23	-.23554005E+04
6140ib配置, 4*Intel Xeon Gold 6140 (18 Cores, 2.30 GHz) 384 G RAM	72	2080	23	-.23554005E+04
6140ib配置, 4*Intel Xeon Gold 6140 (18 Cores, 2.30 GHz) 384 G RAM	36	2456	23	-.23554005E+04
6140ib配置, 4*Intel Xeon Gold 6140 (18 Cores, 2.30 GHz) 384 G RAM	18	5005	23	-.23554005E+04
7702配置, 2*AMD EPYC 7702 (64 Cores, 256MB Cache, 2.0 GHz) 256 G RAM	32	5034	23	-.23554005E+04
7702配置, 2*AMD EPYC 7702 (64 Cores, 256MB Cache, 2.0 GHz) 256 G RAM	64	3663	22	-.23554005E+04
7702配置, 2*AMD EPYC 7702 (64 Cores, 256MB Cache, 2.0 GHz) 256 G RAM	128	4401	23	-.23554005E+04
7502配置, 2*AMD EPYC 7502 (32 Cores, 128MB Cache, 2.5 GHz) 256 G RAM	32	5290	23	-.23554005E+04
7502配置, 2*AMD EPYC 7502 (32 Cores, 128MB Cache, 2.5 GHz) 256 G RAM	64	4176	22	-.23554005E+04

节点	CPU 配置	Elapsed time (s)	scf	E0 in OSZICAR
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

节点	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
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

节点	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 核 2.5GHz, 768GB 内存	8/8	1214.461	23	-.23554005E+04

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