从头开始用 VASP 做结构优化

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VASP 输入文件解读

POSCAR: 晶体结构文件

获取晶体结构I

Inorganic Crystal Structure Database: 实验结构

• ICSD				w	relcome to ICSD W	eb. IP auth	enticated (222.29.1	56.45). Peking Univ				FIZ	Close ses
Login		Basic Search & Retrieve									Search Action		
Loginid:		Bibliography										Run Query	Clear Que
Password:		Authors							Year of Publication				
Login Personalized		Title of Journal										Search Summary Basic Search:	
Lost	Personalize											Basic Search:	
password?	account	Title of Article								Query History			
Content Select	tion O	Chemistry								Number of queries: 0			
Experimental Structures only		Composition	Si				Periodi	c Table	Number of Bements	f 1		Clear Qu	ery History
	Structures only	Cell											
All Structure	95	Cell Parameters											
Vavigation		Cell Volume							=		96		
Q Basic search	to d' antoiness	Call Volume							Tolerance	+/-	96		
d man mar	THE SECURITY	Symmetry											
Advanced search & retrieve		Space Group Symbol			Space Group Number	227							
a, Bibliography	у	ayında			realizer								
D, Cell		Crystal System		-	Centering								
a, Chemistry		Exp. Info. & Ref. I	Data										
a, Symmetry		New Data Only											
Q, Crystal Che	mistry	PDF Number					Temperature			К	*		
a Structure Ty	pe												
Q Experimental Information		ICSD Collection Code					Pressure			MPa	*		
B, DB Info													
Query Manage	ement			Clear Basic	Search			Count Basic Searc	h				
Manage Qu	eries												
List Combin	ned Queries												
5. Create Com	bined Query												

Figure 1: ICSD 搜索页面

获取晶体结构 II

AFLOW: Duke 材料基因组学数据库

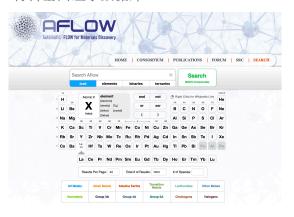


Figure 2: AFLOW 搜索页面

获取晶体结构 III

Materials Project: 基于 pymatgen 的材料基因组学数据库



Figure 3: MaterialsProject 搜索页面

执行 VASP 计算

创建运算目录

▶ 教学一号

```
$ ls
POSCAR POTCAR INCAR KPOINTS sc_run_vasp.sh
$ mkdir session-1/
$ cp POSCAR POTCAR INCAR KPOINTS session-1/
$ cp sc_run_vasp.sh session-1/
$ cd session-1/
```

► TMC PC

```
$ ls
Documents Downloads tests ...
$ mkdir -p tests/YOUR_NAME
$ cp POSCAR POTCAR INCAR KPOINTS tests/YOUR_NAME
$ cd tests/YOUR NAME
```

运行 VASP I

确认 vasp 可执行程序的位置: which

▶ 教学一号

```
$ which vasp_std
$ module load vasp/5.4.4-intel18.0
$ which vasp_std
/nfs-share/software/vasp/intel18.0/bin/vasp_std
```

► TMC PC

```
$ which vasp_std
/home/dft003/software/vasp.5.4.4/bin/vasp_std
```

运行 VASP II

为什么第一次 which 的结果不同?

在教学一号上

```
$ echo $PATH
/nfs-share/software/vasp/intel18.0/bin/:
/nfs-share/software/module/bin:/usr/local/bin:/usr/bin:
```

运行 VASP III

```
$ cat sc run vasp.sh
                             #解释器
#!/usr/bin/env bash
#SBATCH -A 150xxxxxxx
                             # 学号
#SBATCH --nodes=1
                             # 每个任务用 2 个核心
#SBATCH -c 2
#SBATCH --partition=compute # 指定计算分区
                             # 任务名
#SBATCH -J test
#SBATCH -o stdout
module load intel/2018.0 # 载入 Intel 编译器环境变量
module load vasp/5.4.4-intel18.0 # 载入 VASP 环境变量 (PATH)
mpirun -np 2 vasp std
```

运行 VASP IV

▶ 教学一号

```
$ sbatch sc_run_vasp.sh
Submitted batch job xxxx
$ watch -n 1 stdout
```

► TMC PC

```
$ mpirun -np 2 vasp_std > out &
$ watch -n 1 out
```

解读结构优化过程