

从头开始用 VASP 做结构优化

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POSCAR: 晶体结构文件

获取晶体结构 I

Inorganic Crystal Structure Database: 实验结构

 **Welcome to ICSD Web. IP authenticated (222.29.156.45), Peking Univ** FZ Karlsruhe | Contact
Close session

Login LogInId: <input type="text"/> Password: <input type="password"/> <input type="button" value="Login Personalized"/> <input type="button" value="Lost password?"/> <input type="button" value="Personalize account"/>	Basic Search & Retrieve Bibliography Authors: <input type="text"/> Year of Publication: <input type="text"/> Title of Journal: <input type="text"/> Title of Article: <input type="text"/>	Search Action <input type="button" value="Run Query"/> <input type="button" value="Clear Query"/> Search Summary Basic Search: - Query History Number of queries: 0 <input type="button" value="Clear Query History"/>
Content Selection <input checked="" type="radio"/> Experimental Structures only <input type="radio"/> Theoretical Structures only <input type="radio"/> All Structures	Chemistry Composition: <input type="text"/> <input type="button" value="Periodic Table"/> Number of Elements: <input type="text" value="1"/> Cell Cell Parameters: <input type="text"/> Cell Volume: <input type="text"/> Tolerance +/-: <input type="text"/> %	
Navigation <input type="button" value="Q Basic search & retrieve"/> Advanced search & retrieve <input type="button" value="Q Bibliography"/> <input type="button" value="Q Cell"/> <input type="button" value="Q Chemistry"/> <input type="button" value="Q Symmetry"/> <input type="button" value="Q Crystal Chemistry"/> <input type="button" value="Q Structure Type"/> <input type="button" value="Q Experimental Information"/> <input type="button" value="Q DB Info"/> Query Management <input type="button" value="Manage Queries"/> <input type="button" value="List Combined Queries"/> <input type="button" value="Create Combined Query"/>	Symmetry Space Group Symbol: <input type="text"/> Space Group Number: <input type="text" value="227"/> Crystal System: <input type="text"/> Centering: <input type="text"/> Exp. Info. & Ref. Data New Data Only: <input type="checkbox"/> PDF Number: <input type="text"/> Temperature: <input type="text"/> K ICSD Collection Code: <input type="text"/> Pressure: <input type="text"/> MPa <input type="button" value="Clear Basic Search"/> <input type="button" value="Count Basic Search"/>	

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

AFLOW
Automatic - FLOW for Materials Discovery

HOME | CONSORTIUM | PUBLICATIONS | FORUM | SRC | SEARCH

Search AFLOW

Search (93375 Compounds)

lead elements binaries ternaries

Atomic # element
mass formula
(element) [Tol] (crystal)
(oxide) (oxide)

and not
or xor
()

Right Click for Wikipedia Link

Results Per Page: 40 Total # of Results: 1000 # of Species:

All Metals Alkali Metals Alkaline Earths Transition Metals Lanthanides Other Metals
Nonmetals Group 3A Group 4A Group 5A Chalcogens Halogens

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

The screenshot displays the Materials Project search page. At the top, there is a navigation bar with links for Home, About, Apps, Documentation, API, Tutorials, and Dashboard. Below this is a search bar with the text "Search for materials information by chemistry, composition, or property". The main content area is titled "Explore Materials" and features a "Q by Elements" dropdown menu with a search input field containing "Na-O". A periodic table of elements is shown, with elements color-coded by groups. To the right of the periodic table, there are several filters and search options: "Number of elements" (e.g., <4 or >2 & <6), "excluded elements" (e.g., Br), "Material Tags" (e.g., Inorganic), "Band Gap (eV)" (0 to 10), "Energy Above Hull" (0 to 6), and "Formation Energy" (-4 to 4). The interface is clean and modern, with a dark blue header and a light gray background.

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
#!/usr/bin/env bash                                # 解释器
#SBATCH -A 150xxxxxxx                               # 学号
#SBATCH --nodes=1                                    # 使用一个节点
#SBATCH -c 2                                          # 每个任务用 2 个核心
#SBATCH --partition=compute                          # 指定计算分区
#SBATCH -J test                                       # 任务名
#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
```

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