#### 从头开始用 VASP 做结构优化

张旻烨 王越超 许熙 栾东

## 登入 Linux

# 编辑文件

## VASP 输入文件解读

POSCAR: 晶体结构文件

#### 获取晶体结构I

#### 实验结构: Inorganic Crystal Structure Database

• ICSD				w	relcome to ICSD W	eb. IP auth	enticated (222.29.1	56.45). Peking Univ				FIZE	Carisruhe   Co Close se	
Login		Basic Search & Retrieve								Search Action				
Loginid:		Bibliography										Run Query	Clear Qu	ery
Password:	assword: A								Year of Publicatio	Year of Publication				
Login Personalized		Title of Journal										Search Summary		
Login Personatoso												Basic Search:		
password? account		Title of Article									Query History			
Content Selection (2)		Chemistry										Number of queries: 0		
Experimental Structures only		Composition	Si				Periodic	c Table	Number of Bements	1		Clear Qu	ary History	
		Cell												
All Structure		Cell Parameters												
Navigation														
Q. Basic search & retrieve		Cell Volume							Tolerance	+/-	96			
CL BASIC SHAPE	1 & RECTIONS	Symmetry												
Advanced search & retrieve		Space Group Symbol			Space Group Number	227								
<ul> <li>Bibliography</li> </ul>	,	ojiinu			realized									
Q Cell		Crystal System		-	Centering									
@ Chemistry		Exp. Info. & Ref. I	Data											
@ Symmetry		New Data Only												
Q Crystal Cher	nistry	PDF Number					Temperature			К	*			
Q Structure Type														
Q Experimental Information		ICSD Collection Code					Pressure			MPa	*			
Q DB Info														
Query Management				Clear Basic	Search			Count Basic Search						
Œ Manage Que	ries													
III List Combine	ed Queries													
Δ. Create Comi	bined Query													

Figure 1: ICSD 搜索页面

## 获取晶体结构 Ⅱ

计算结构:

**AFLOW** 

#### 获取晶体结构 III

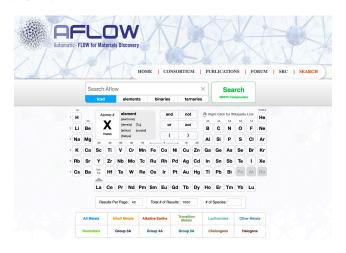


Figure 2: AFLOW 搜索页面

#### 获取晶体结构 IV

Materials Project, 基于 pymatgen



Figure 3: MaterialsProject 搜索页面

## 执行 VASP 计算

## 解读结构优化过程