

# 从头开始用 VASP 做结构优化

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# 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

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

<b>Login</b> 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"/>	<b>Basic Search &amp; Retrieve</b> <b>Bibliography</b> Authors: <input type="text"/> Year of Publication: <input type="text"/> Title of Journal: <input type="text"/> Title of Article: <input type="text"/> <b>Chemistry</b> Composition: <input type="text"/> <input type="button" value="Periodic Table"/> Number of Elements: <input type="text" value="1"/> <b>Cell</b> Cell Parameters: <input type="text"/> Cell Volume: <input type="text"/> Tolerance +/-: <input type="text"/> % <b>Symmetry</b> Space Group Symbol: <input type="text"/> Space Group Number: <input type="text" value="227"/> Crystal System: <input type="text"/> Centering: <input type="text"/> <b>Exp. Info. &amp; Ref. Data</b> 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"/>	<b>Search Action</b> <input type="button" value="Run Query"/> <input type="button" value="Clear Query"/> <b>Search Summary</b> Basic Search: - <b>Query History</b> Number of queries: 0 <input type="button" value="Clear Query History"/>
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**Content Selection**  
☒ Experimental Structures only  
☐ Theoretical Structures only  
☐ All Structures

**Navigation**  
  
**Advanced search & retrieve**  
  
  
  
  
  
  
  
  
**Query Management**

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

The screenshot displays the AFLOW website, which is dedicated to materials discovery. The header features the AFLOW logo and navigation links: HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below the header is a search bar with the text "Search AfLOW" and a "Search" button indicating 69375 compounds. A filter bar below the search bar allows users to select between "icad", "elements", "binaries", and "ternaries". The main content area features a periodic table of elements. A pop-up window for element "X" shows its properties: Atomic #, element name, [electrons], [density], [T<sub>u</sub>], [lattice], [crystal], [mass], and [Debye]. To the right of the periodic table are logical operators: "and", "not", "or", "xor", and parentheses. Below the periodic table, there are filters for "Results Per Page" (set to 40), "Total # of Results" (1000), and "# of Species". At the bottom, there are buttons for various material categories: All Metals, Alkali Metals, Alkaline Earths, Transition Metals, Lanthanides, Other Metals, Nonmetals, Group 3A, Group 4A, Group 5A, Chalcogens, and Halogens.

Figure 2: AFLOW 搜索页面



# 获取晶体结构 IV

Materials Project, 基于 pymatgen

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 features a periodic table of elements, with a search bar above it labeled "Explore Materials" and "Advanced Search Syntax". The search bar has a dropdown menu set to "by Elements" and a search input field containing "Na-O". To the right of the periodic table, there are three search filters: "# of elements" (with a value of 4), "excluded elements" (with a value of Br), and "Material Tags" (with a value of Imagite). Below these filters are three sliders: "Band Gap (eV)" (ranging from 0 to 10), "Energy Above Hull" (ranging from 0 to 6), and "Formation Energy" (ranging from -4 to 4).

Figure 3: MaterialsProject 搜索页面

# 执行 VASP 计算

## 解读结构优化过程