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

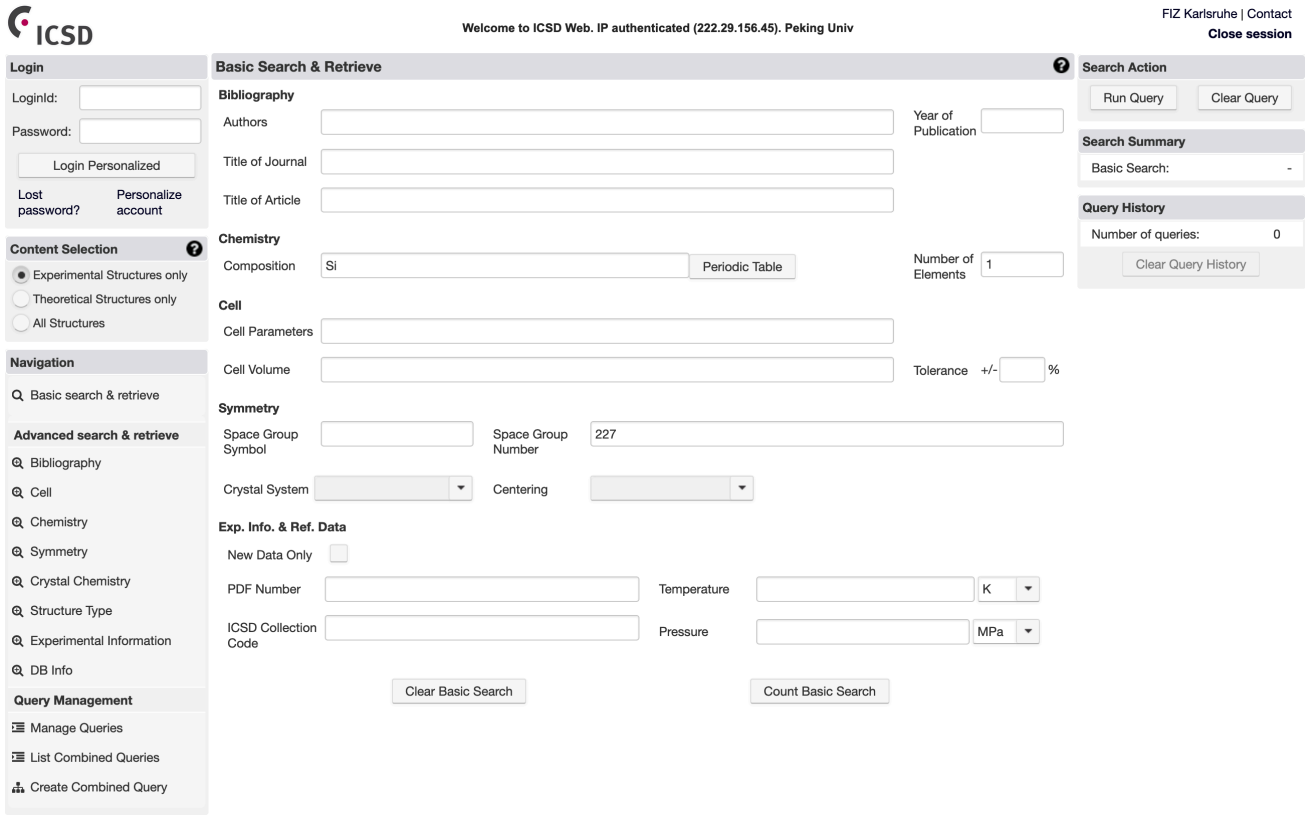

Figure 1: ICSD 搜索页面

获取晶体结构 II

计算结构:

AFLOW

获取晶体结构 III

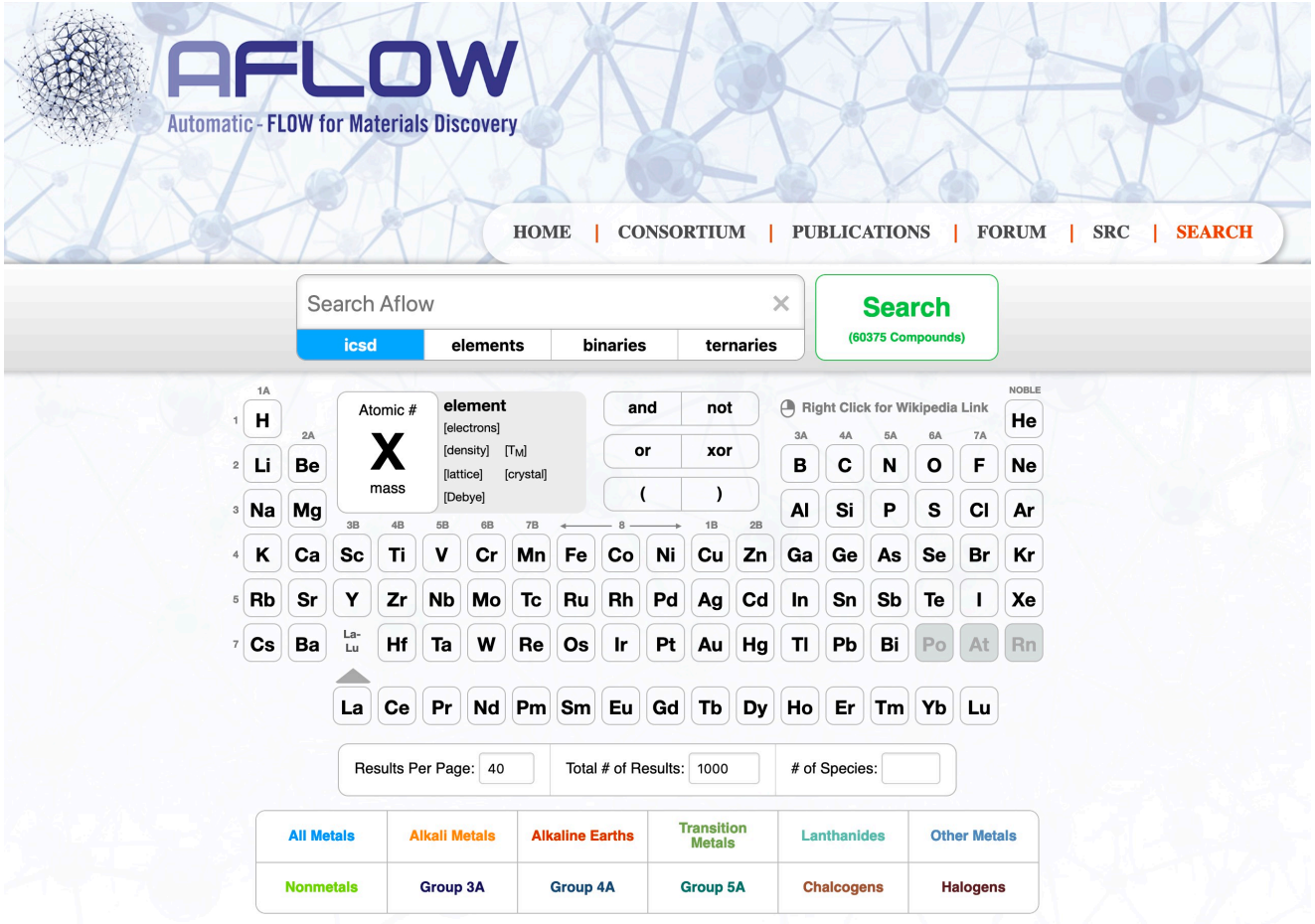

Figure 2: AFLOW 搜索页面

获取晶体结构 IV

Materials Project, 基于 `pymatgen`

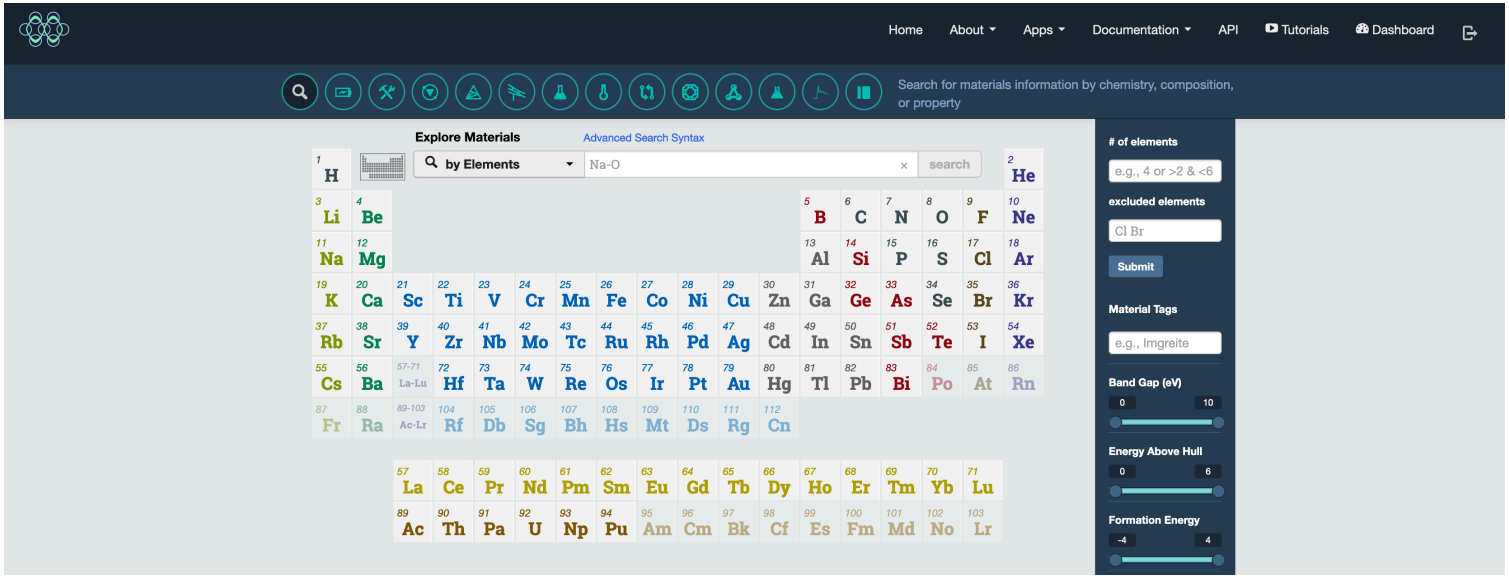

Figure 3: MaterialsProject 搜索页面

执行 VASP 计算

解读结构优化过程