# VASP入门培训基础

易文才

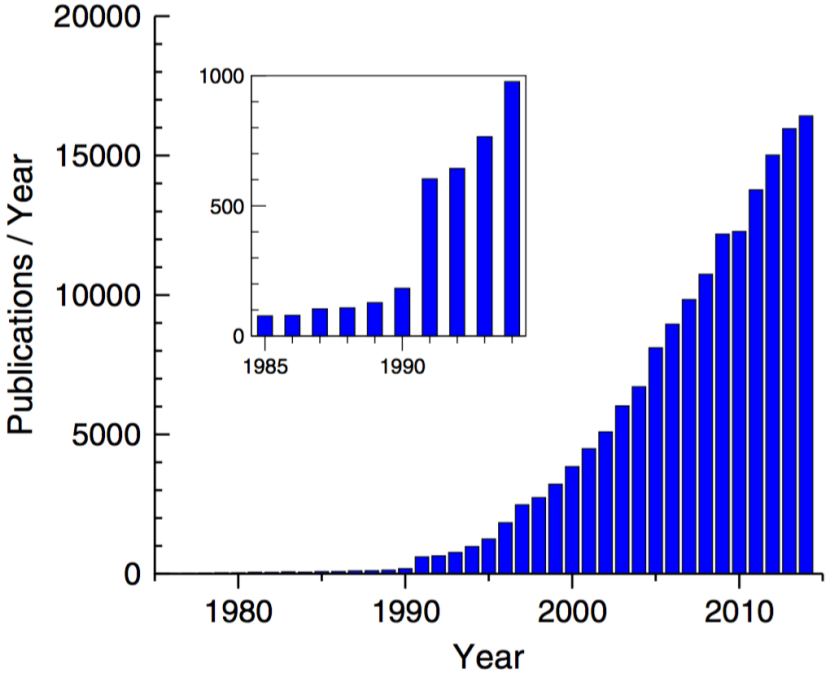
# 基于DFT方法的文章发表数量

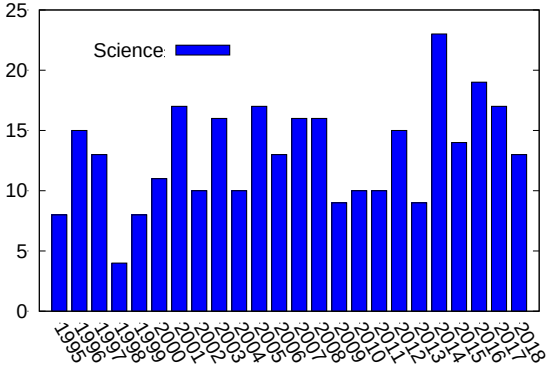
REVIEWS OF MODERN PHYSICS, VOLUME 87, JULY–SEPTEMBER 2015

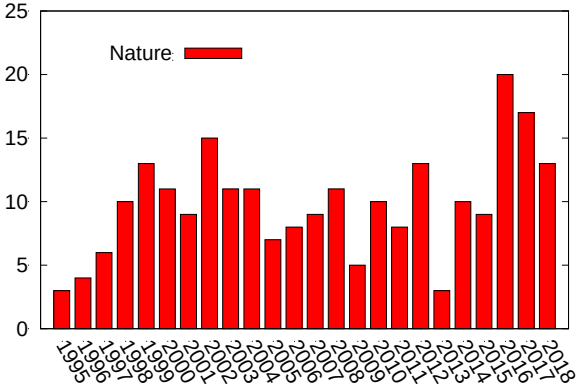
**Density functional theory: Its origins, rise to prominence, and future**

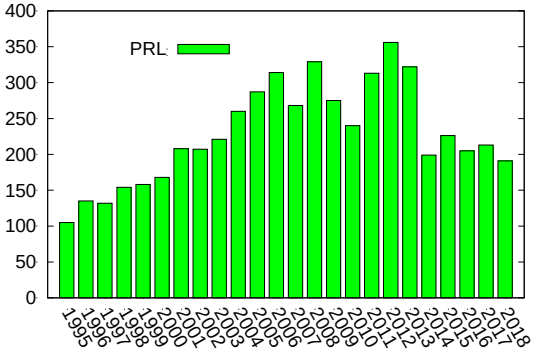
R. O. Jones*

*Peter-Grünberg-Institut PGI-1 and German Research School for Simulation Sciences, Forschungszentrum Jülich, D-52425 Jülich, Germany*



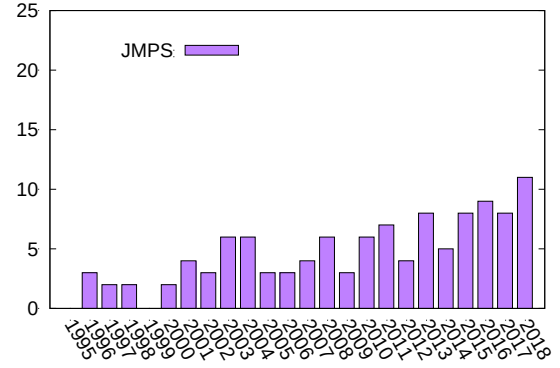
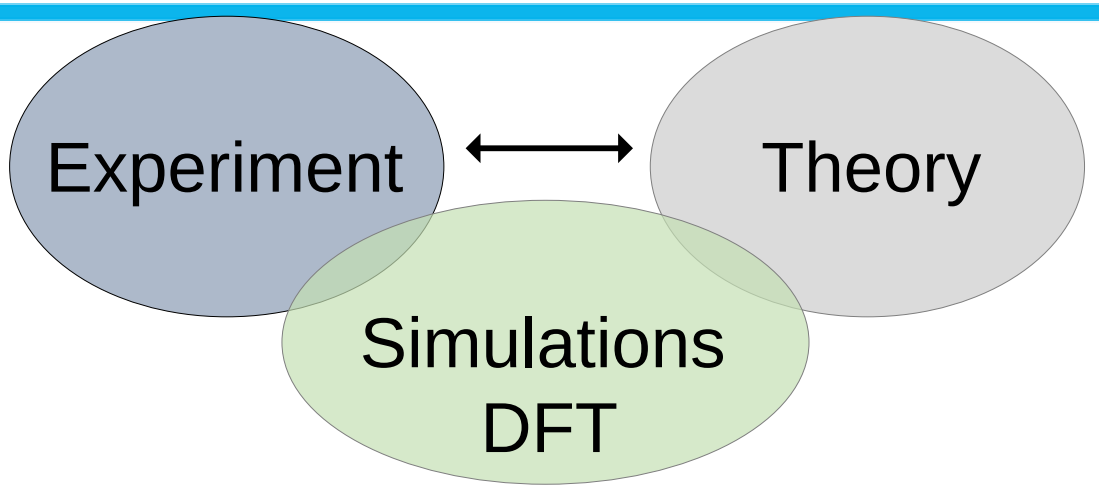




FIG. 1 (color online). Number of publications per year (1975–2014) on topics ("density functional" or "DFT"), according to the Web of Science Core Collection (February 2015). The inset shows data near 1990 on an expanded scale. The number of publications depends on the precise search criteria, but the overall picture is unchanged. From Mavropoulos, 2015.

# DFT理论模拟的优势




—加深认识

- 材料原子层次上的性质，比如电子结构等
- 解释催化等反应机理等，比如过渡态研究

—实用价值

- 指导实验研究--可以减少实验试错次数和降低成本
- 能够预测实验条件无法实现的相关材料的结构和性质(超高温、高压)

—低成本

# 超高热导率材料

理论驱动实验验证的实例

measured. In 2013, a stunning prediction was made that $\kappa_{BAs}$ might be 10 times as high and approach $\kappa_{Diamond}$ (*2*). Testing such predictions (*2*, *3*) required BAs crystals of unprecedented quality, which launched a flurry of experimental efforts. Reports by Kang *et al.* (*4*) on page 575, Tian *et al.* (*5*) on page 582, and Li *et al.* (*6*) on page 579 of this issue describe the synthesis of small yet superb crystals of BAs and the measurement of $\kappa_{BAs}$ values of ~1100 W/m·K. These results verify the essence of the predictions (*2*, *3*) and earn BAs long-overdue recognition as an ultrahigh-κ material.

L.Lindsay et al.,*PRL.*111, 025901 (2013).

*RESEARCH*

THERMAL CONDUCTIVITY

## High thermal conductivity in cubic boron arsenide crystals

Sheng Li[1]*, Qiye Zheng[2]*, Yinchuan Lv[3], Xiaoyuan Liu[1], Xiqu Wang[4], Pinshane Y. Huang[2], David G. Cahill[2]†, Bing Lv[1]†

The high density of heat generated in power electronics and optoelectronic devices is a

*RESEARCH*

REPORT

THERMAL CONDUCTIVITY

## Experimental observation of high thermal conductivity in boron arsenide

*RESEARCH*

THERMAL CONDUCTIVITY

## Unusual high thermal conductivity in boron arsenide bulk crystals

Fei Tian[1]*, Bai Song[2]*, Xi Chen[3]*, Navaneetha K. Ravichandran[4], Yinchuan Lv[5], Ke Chen[2], Sean Sullivan[3], Jaehyun Kim[6], Yuanyuan Zhou[6], Te-Huan Liu[2], Miguel Goni[7], Zhiwei Ding[2], Jingying Sun[1], Geethal Amila Gamage Udalamatta Gamage[1], Haoran Sun[1], Hamidreza Ziyaee[8], Shuyuan Huyan[1], Liangzi Deng[1], Jianshi Zhou[1], Aaron J. Schmidt[7], Shuo Chen[1], Ching-Wu Chu[1,9], Pinshane Y. Huang[10], David Broido[4]†, Li Shi[3,6]†,

# 金属氢

## First Sample of Solid Metallic Hydrogen Lost

By Akshitha Ramachandran , Crimson Staff Writer

March 7, 2017

A month after two Harvard physicists published results detailing the synthesis of the first-ever sample of solid metallic hydrogen, the researchers have lost the sample after trying to further analyze it.

In late January, Isaac F. Silvera and Ranga P. Dias—a Harvard physics professor and postdoctoral researcher respectively—published their discovery of the potential "superconductor," which could transform the way electricity is conducted. In a paper in the journal Science, they wrote that under extreme pressure and at low temperatures they were able to transform a hydrogen sample into a solid state—a discovery that has eluded scientists for over 80 years.

The team decided to keep the single sample they created in the diamond anvil cell —the apparatus used for the experiment—until their findings were published. After their research was released in Science, they planned on sending the sample to Argonne National Laboratory in Chicago where it could be further studied.

Hig

drogen

Science

REPORTS

P. Dias *et al.*, *Science*
ience.aal1579 (2017).

Obser
metall

0

**Ranga P. Dias and Isaac F. Silvera**

Lyman Laboratory of Physics, Harvard University, Cambridge, MA 02138, USA.

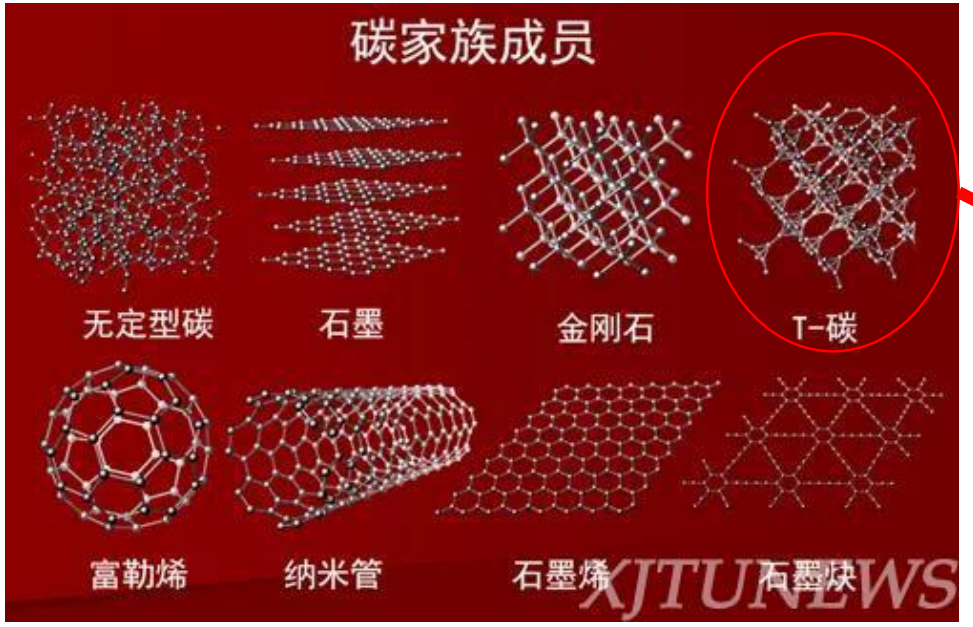
# 超硬材料

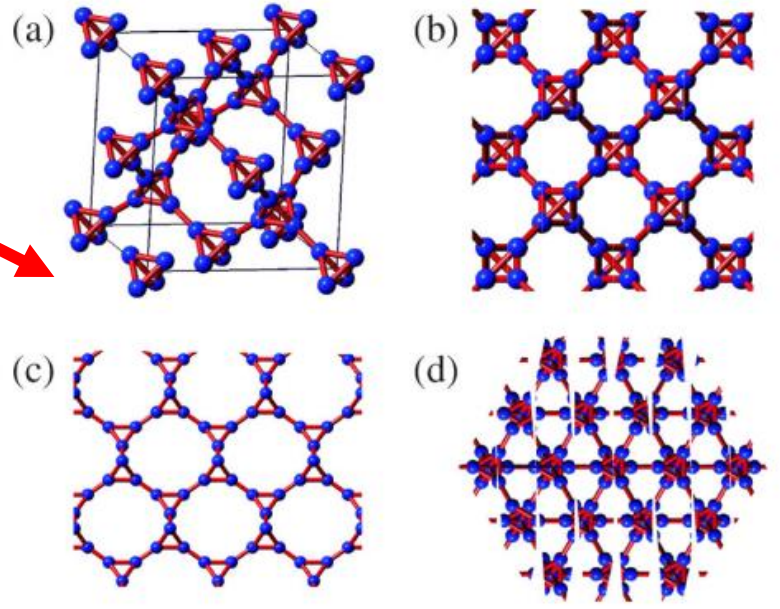
## T-Carbon: A Novel Carbon Allotrope

Xian-Lei Sheng,[1] Qing-Bo Yan,[2] Fei Ye,[2] Qing-Rong Zheng,[1] and Gang Su[1,*]

[1]*College of Physical Sciences, Graduate University of Chinese Academy of Sciences, P.O. Box 4588, Beijing 100049, China*

[2]*College of Materials Science and Opto-Electronic Technology, Graduate University of Chinese Academy of Sciences, P.O. Box 4588, Beijing 100049, China*



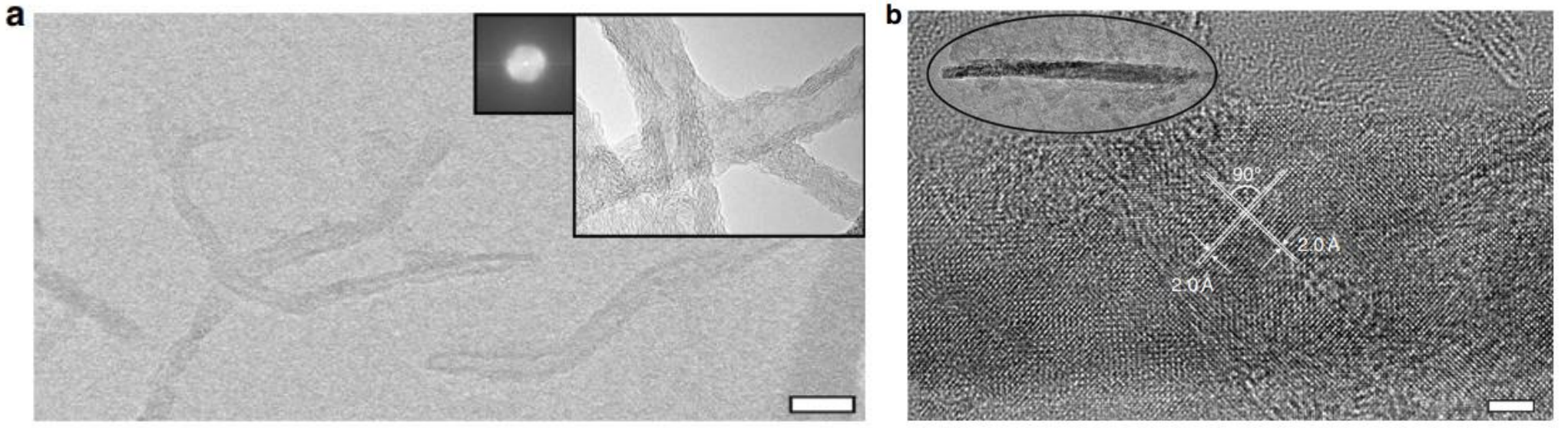

2011年，中国科学院大学研究团队通过理论计算预言了一种新型三维碳结构，并把这种碳的新型同素异形体命名为T-carbon。T-carbon还有一个很鲜明的特点，其密度非常小，约为石墨的2/3，金刚石的一半。T-carbon也具有很高的硬度。由于T-carbon是一个蓬松的碳材料，其内部有很大空间可供利用，如果用于储能材料，其储氢能力不低于7.7wt%。由于上述独特的性能，T-carbon将会在光催化、吸附、储能、航空航天材料等领域拥有广泛的潜在应用。

# 超硬材料

DOI: 10.1038/s41467-017-00817-9 OPEN

## Pseudo-topotactic conversion of carbon nanotubes to T-carbon nanowires under picosecond laser irradiation in methanol

Jinying Zhang[1], Rui Wang[1], Xi Zhu[2], Aifei Pan[3], Chenxiao Han[1], Xin Li[1], Dan Zhao[1], Chuansheng Ma[4], Wenjun Wang[3], Haibin Su[2] & Chunming Niu[1]




2017年西安交大牛春明课题组和新加坡南洋理工大学联合研究团队实验上在瞬间飞秒激光照射下中空的碳纳米管转变为实心的碳纳米棒，碳纳米棒中碳原子之间的连接方式同理论预测的T-carbon完全一致，证明合成了这种结构。

# 实验+理论是材料研发的趋势

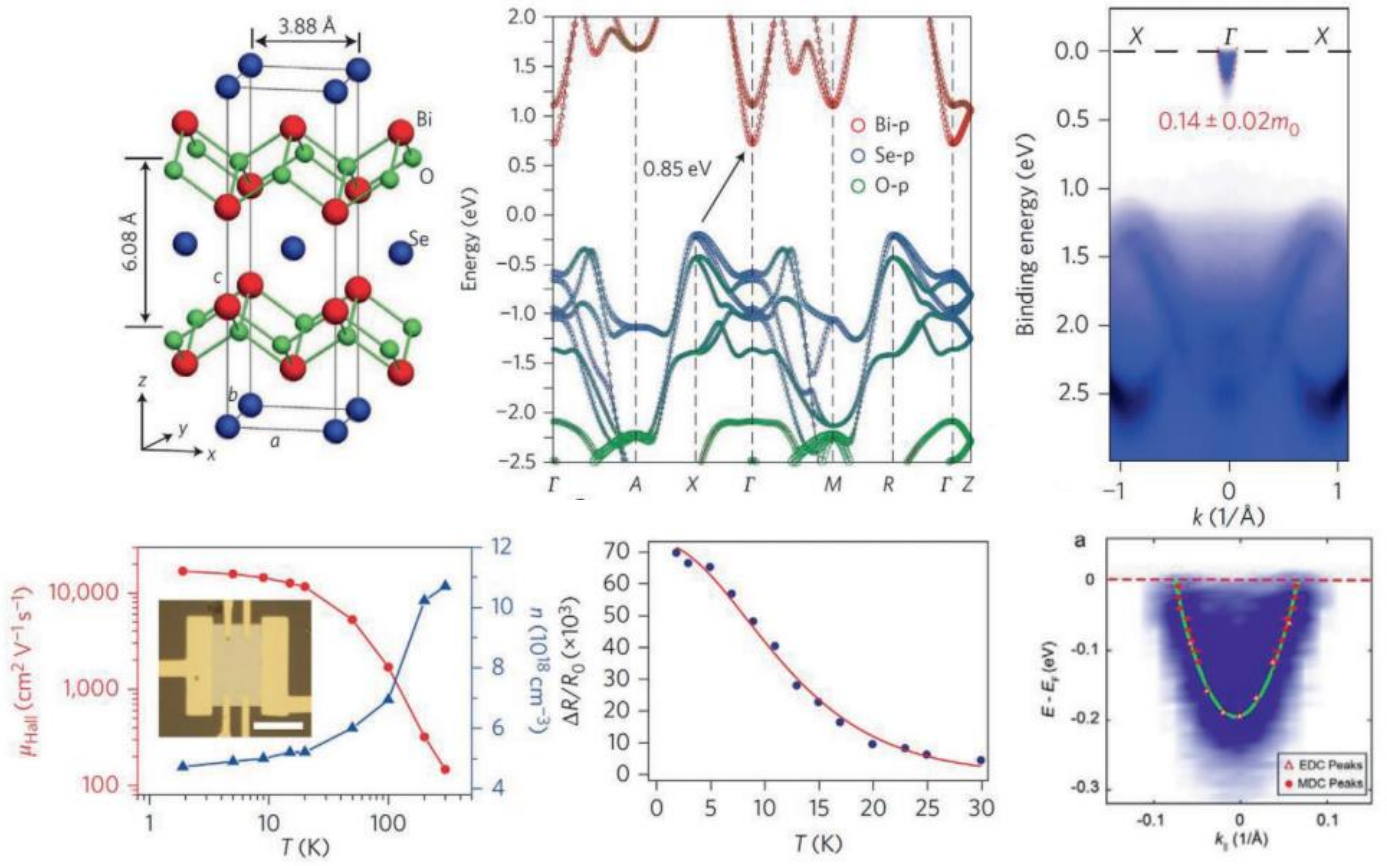
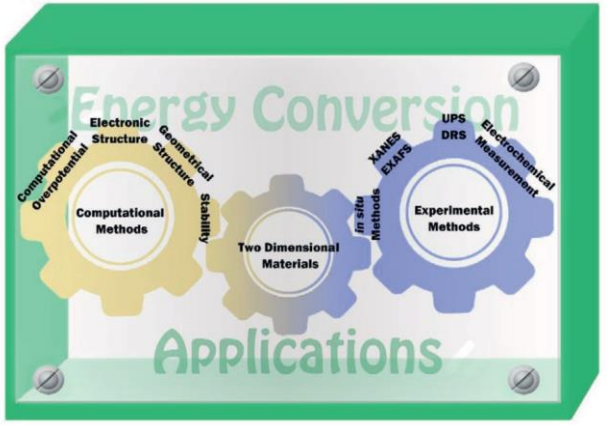



**Figure 6.** a) Atomic structure and b) computed band structure at GGA level of layered $Bi_2O_2Se$. c) Band dispersions of CB after surface K-dosing to lift the chemical potential observed by ARPES. d) Hall mobility ($\mu_{Hall}$, left) and carrier density ($n$, right) as a function of temperature for $Bi_2O_2Se$ nanoplate. e) Temperature-dependent $\Delta R/R_0$ values of SdH oscillations and Lifshitz-Kosevich fitting at 1.28 T. f) Photoemission spectrum and parabolic fitting around Γ point. Reproduced with permission.[146] Copyright 2017, Nature.




实验与材料模拟分别是研究材料性能的两种工具，是两种技术手段，需要公平对待。

研究领域的共性即“不确定性”，也正因此才需要研究。故很多问题，言之有理即可（重复性很关键）。

Zhang, X., Chen, A., Chen, L. and Zhou, Z., 2D Materials Bridging Experiments and Computations for Electro/Photocatalysis. *Advanced Energy Materials*, p.2003841.

**目前代算绝不可取！**

# 热点材料极其研究核心

1、二维气敏材料简介

2、光催化材料简介

3、单原子催化材料简介

4、SERS基底材料简介

5、二维异质结材料简介

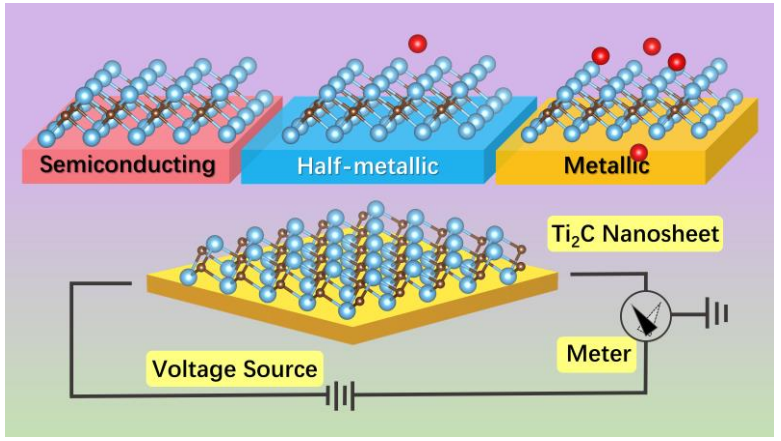
6、钙钛矿（光伏）材料简介

7、电池（电极）材料简介

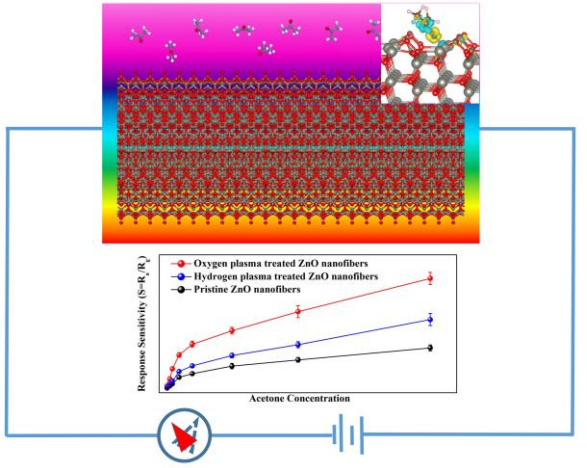
8、含能材料简介

9、热电材料简介

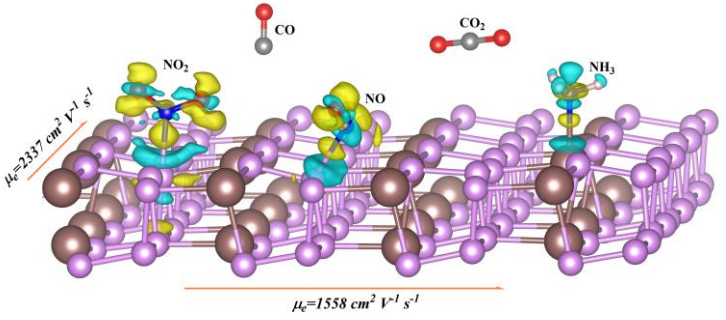
# 二维气敏材料



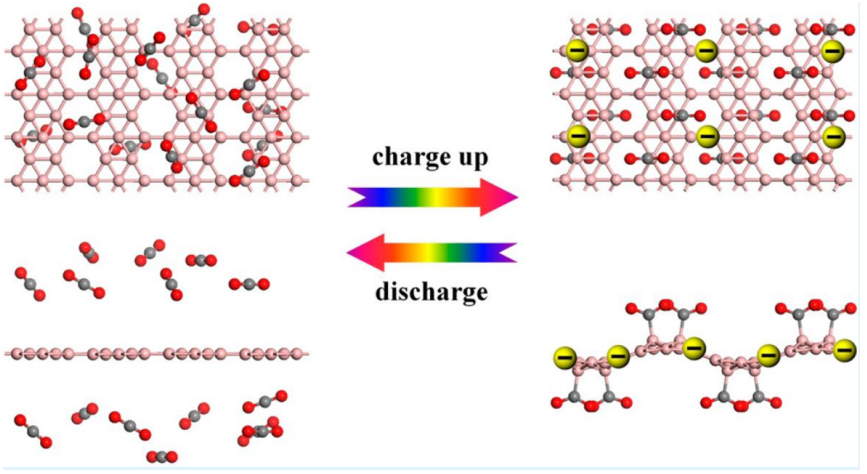

*Appl. Surf. Sci.* 544 (2021): 148925



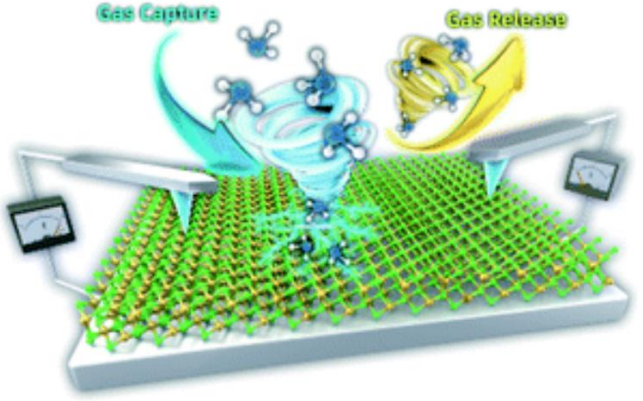

*ACS Appl. Mater. Inter.* 12.20 (2020): 23084-23093




*J. Mater. Chem. C* 7.24 (2019): 7352-7359.



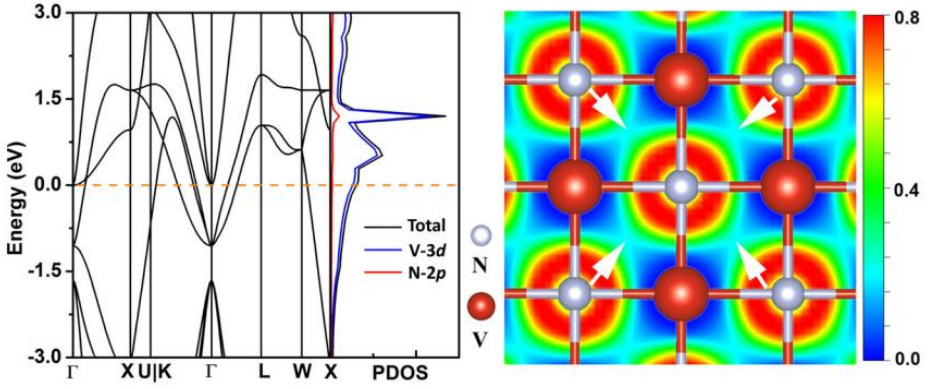

*ACS Appl. Mater. Inter.* 9.23 (2017): 19825-19830



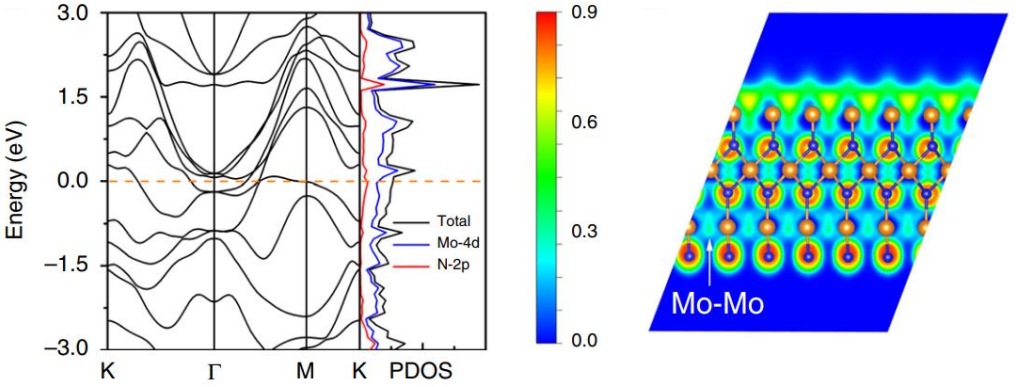

*J. Mater. Chem. A* 8.15 (2020): 7331-7338.

*核心问题：响应灵敏度、气体选择性、可逆性*

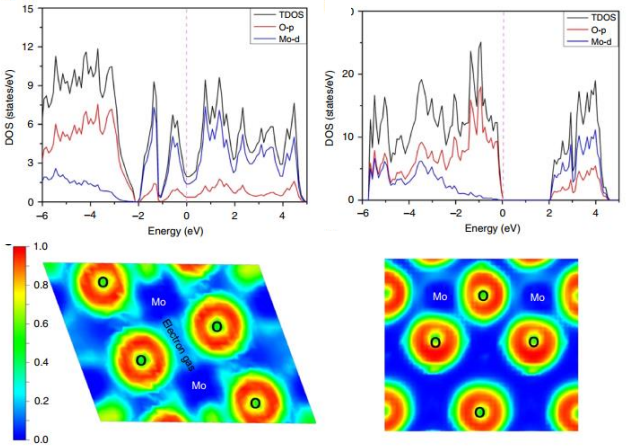
# SERS基底材料



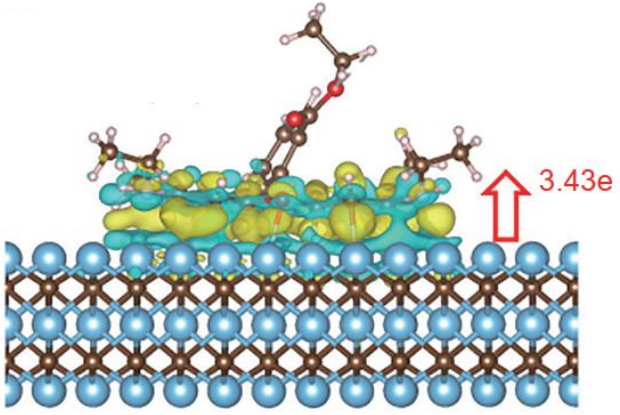

*Nat. Commun.* 12.1 (2021): 1-11.



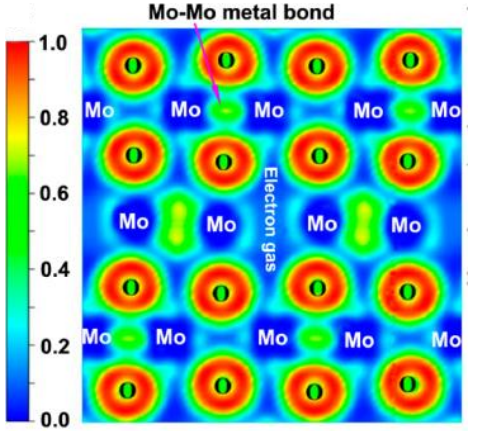

*Nat. commun.* 11.1 (2020): 1-9.




*Nat. Commun.* 8.1 (2017): 1-9.



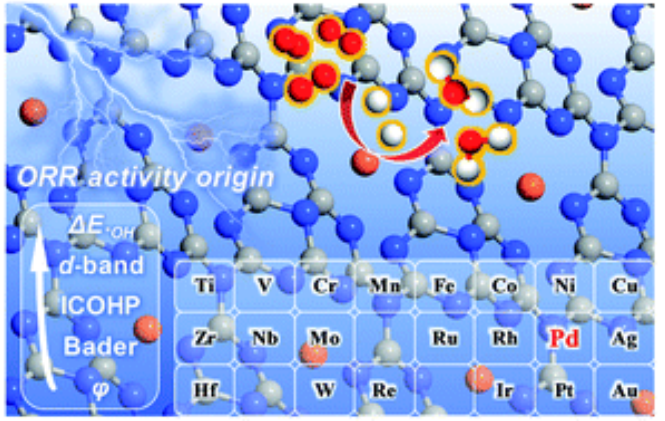

*Sci. China Mater.* 63.5 (2020): 794-805.

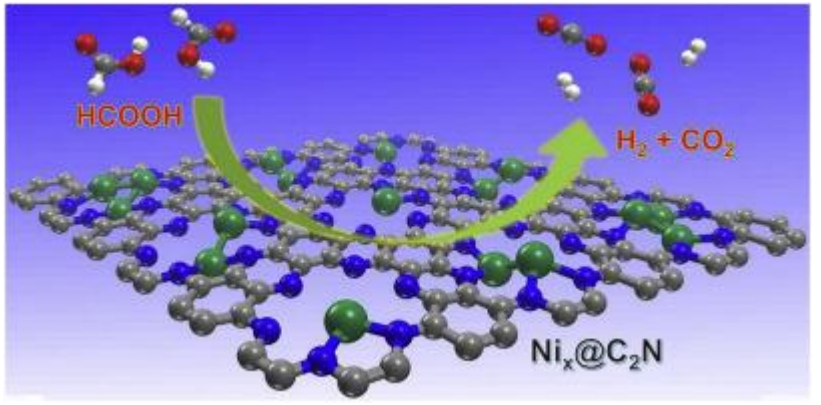



*ACS nano* 14.10 (2020): 13718-13726.

*核心问题：高稳定性、高灵敏响应性、价格低、化学增强与物理增强机制*

# 单原子催化简介

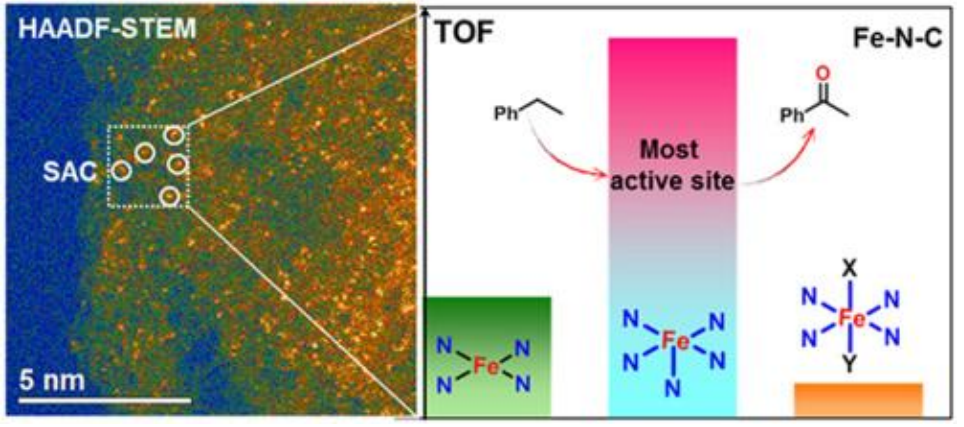


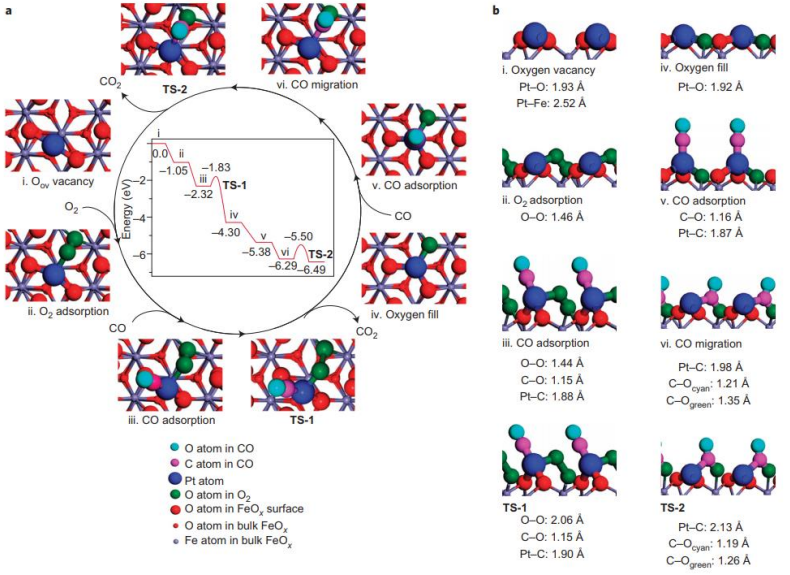

**原理类似戒指镶钻**

*J. Mater. Chem. A* 8.14 (2020): 6555-6563

*J. Power Sources* 413 (2019): 399-407



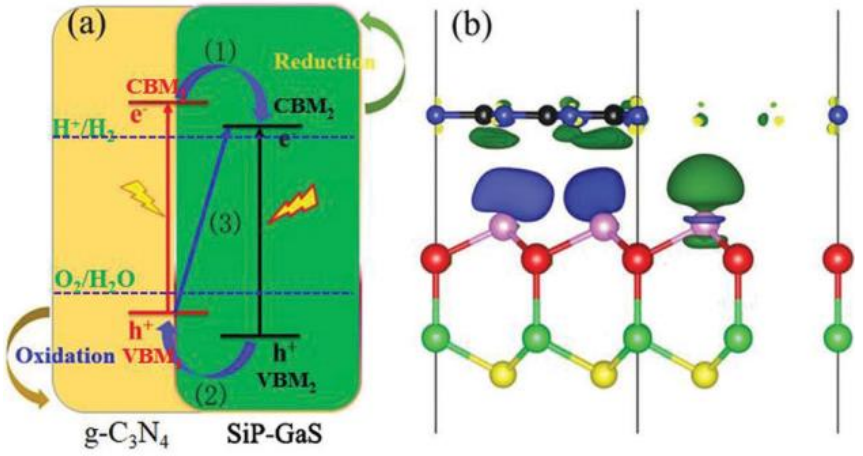

*J. Am. Chem. Soc.* 2017, 139, 31, 10790–10798



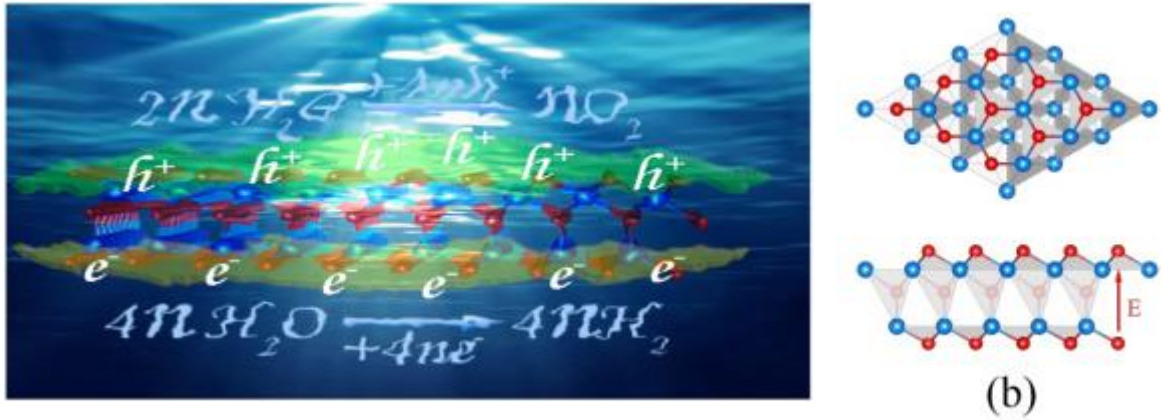

*Nat. Chem.* 3.8 (2011): 634-641

*核心问题：高稳定性、高催化能力、低成本性*

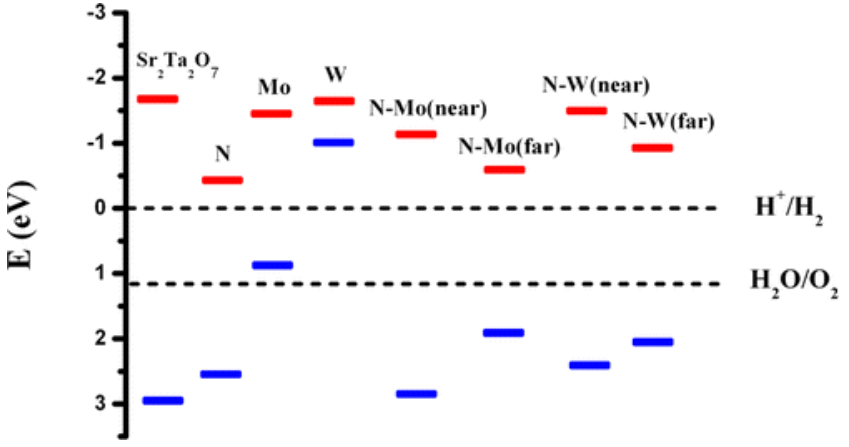
# 光催化材料



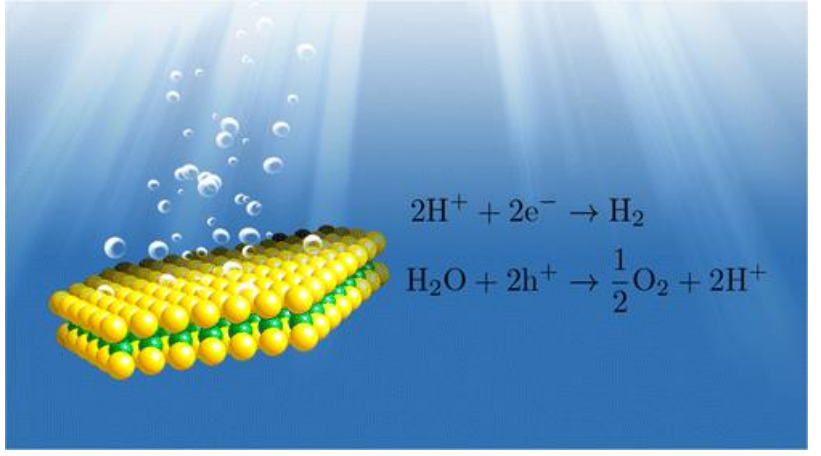

*Phys. Chem. Chem. Phys.* 22.27 (2020): 15649-15657.




*Nano Energy* 51 (2018): 533-538.



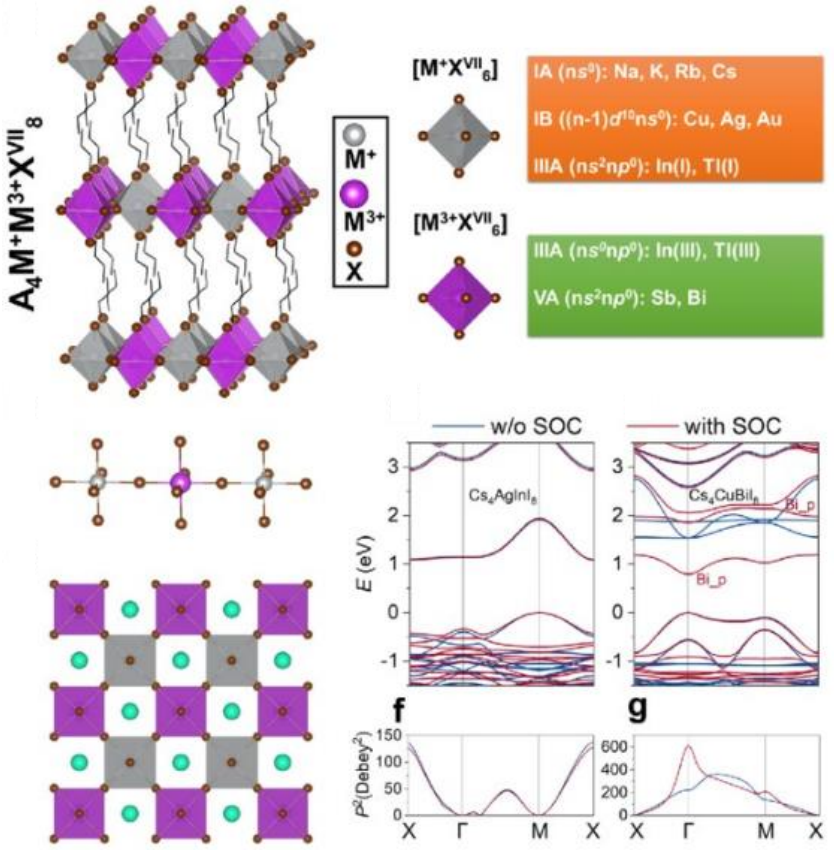

*J. Phys. Chem. C* 2013, 117, 10, 5043–5050



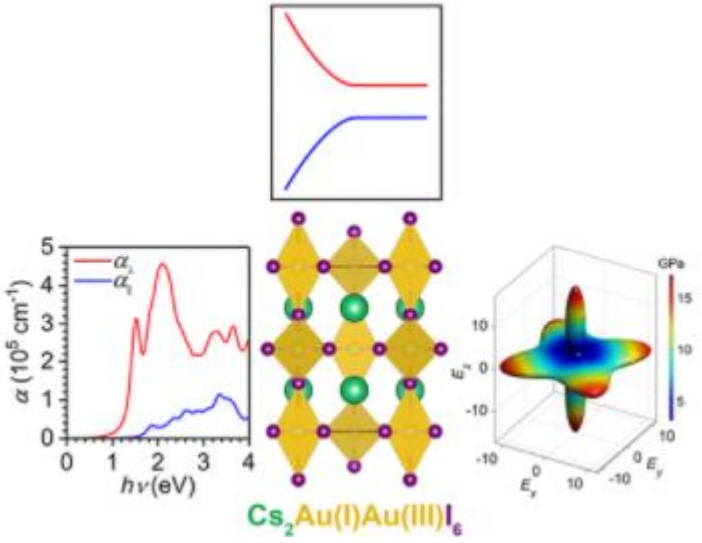

*J. Phys. Chem. Lett.* 2015, 6, 6, 1087–1098

*核心问题：高稳定性、高光吸收效率、带边能级要对齐、激发态难处理*

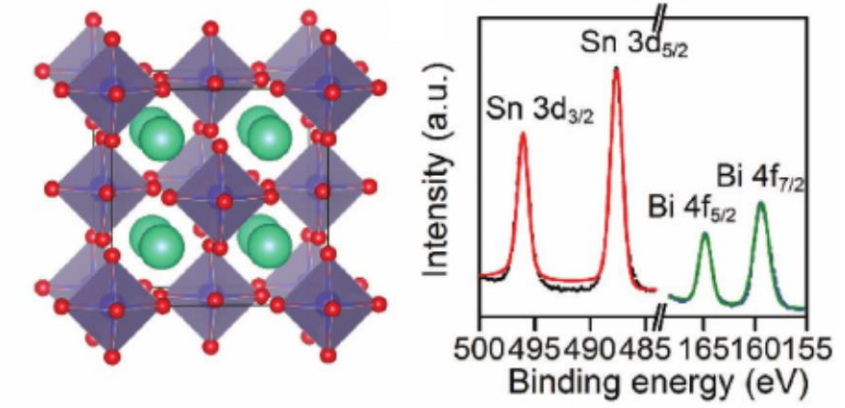
# 钙钛矿（光伏）材料




*ACS Energy Lett.* 5.7 (2020): 2275-2282



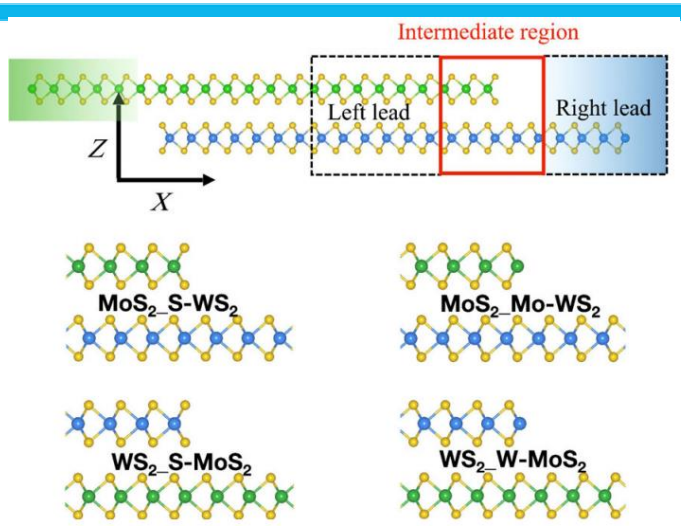

*J. Phys. Chem. Lett.* 10.21 (2019): 6688-6694



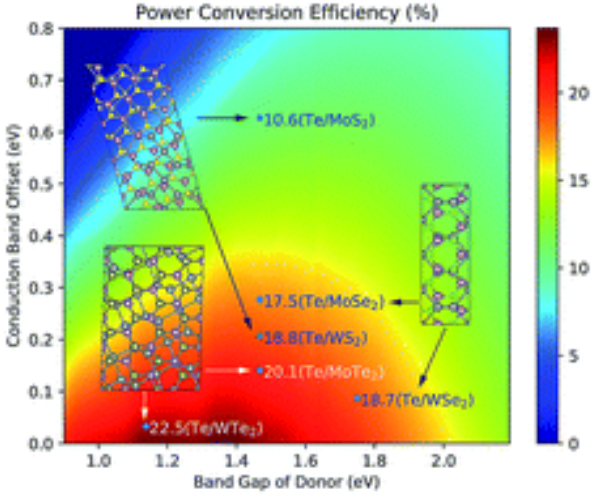

*Adv. Funct. Mater.* 28.29 (2018): 1801131.

*核心问题：高稳定性、高光吸收效率、带边能级要对齐、激发态难处理*

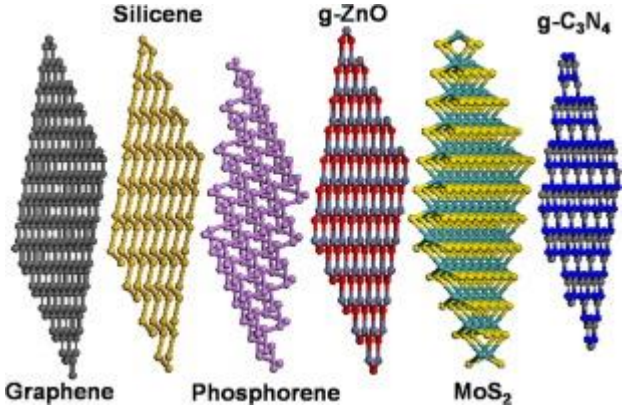
# 二维异质结材料



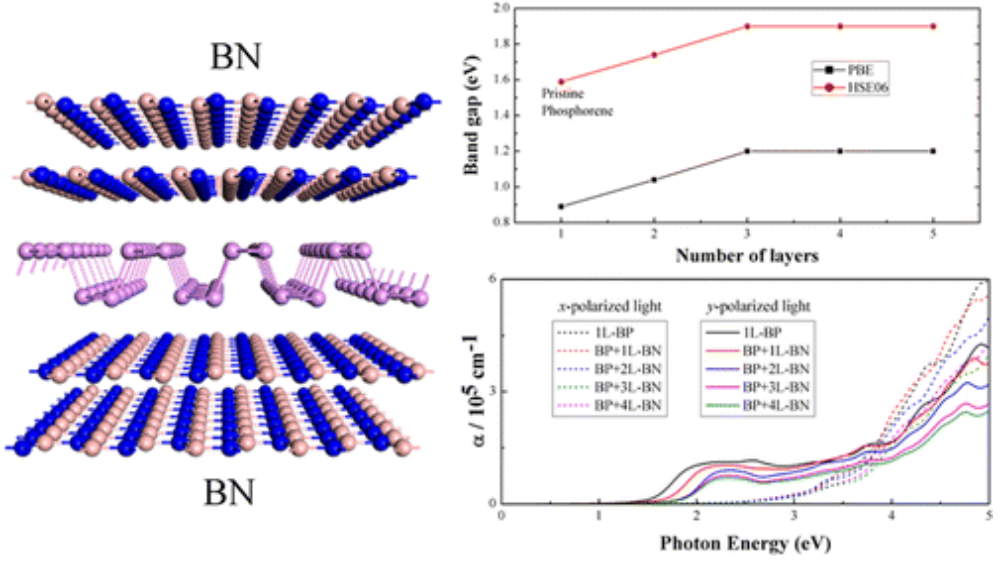

*Nano Research* (2020): 1-8




*J. Mater. Chem. A* 7.13 (2019): 7430-7436



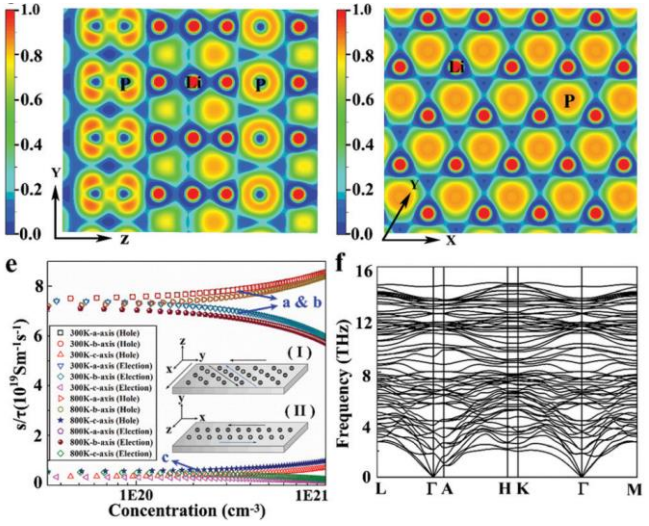

*Comp. Mater. Sci.* 112 (2016): 518-526



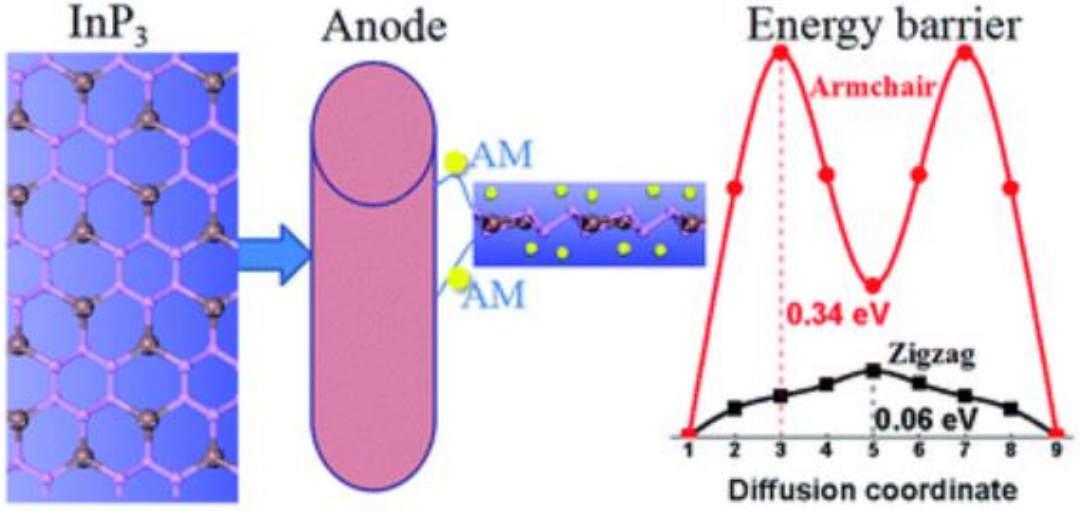

*ACS Appl. Mater. Interfaces* 2015, 7, 42, 23489–23495

*核心问题：晶格匹配，载流子复核时间*

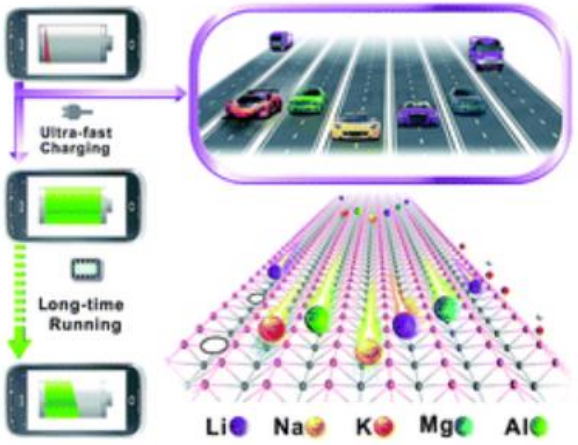
# 电池（电极）材料



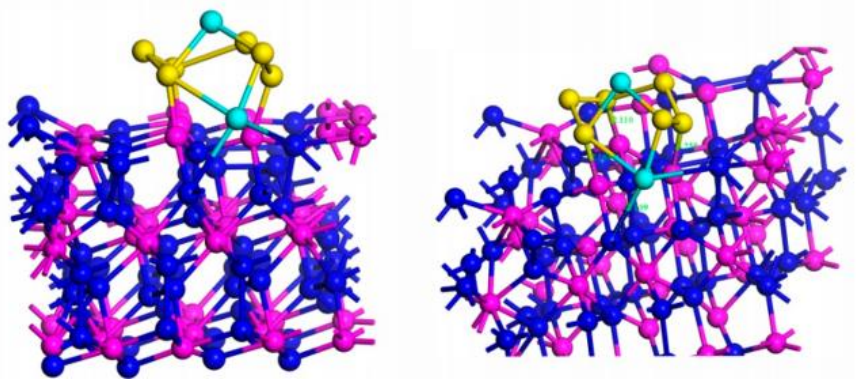

*Phys. Chem. Chem. Phys.* 22.34 (2020): 19172-19177




*J. Mater. Chem. A* 6.8 (2018): 3634-3641



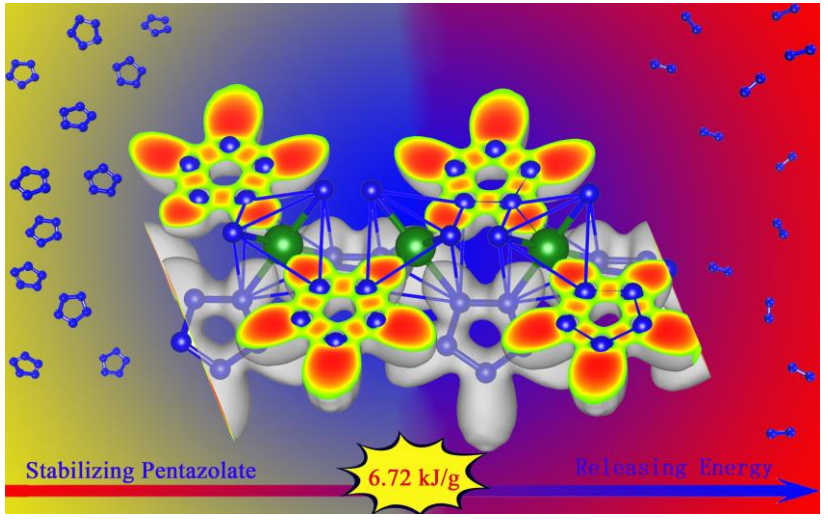

*J. Mater. Chem. A* 5.5 (2017): 2328-2338



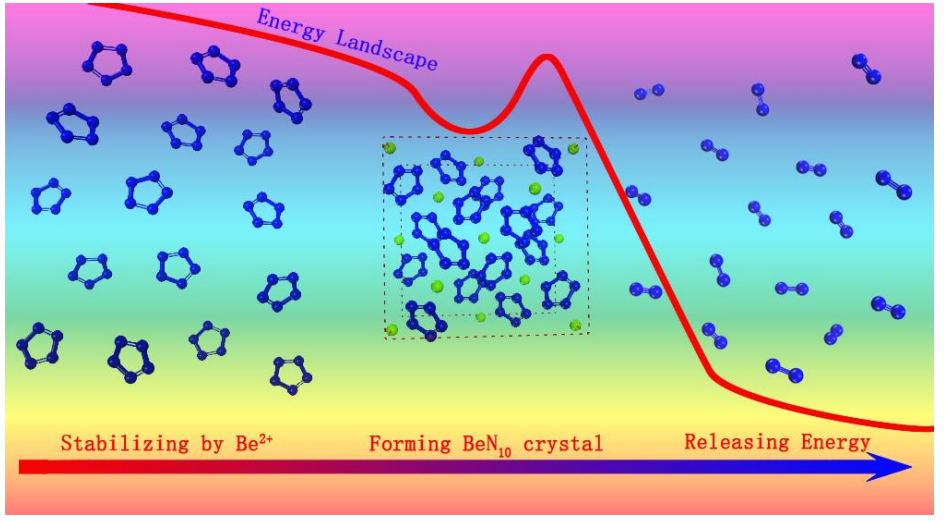
*ACS Nano* 2019, 13, 4, 4731–4741

*核心问题：高稳定性、高容量、优异导电性*

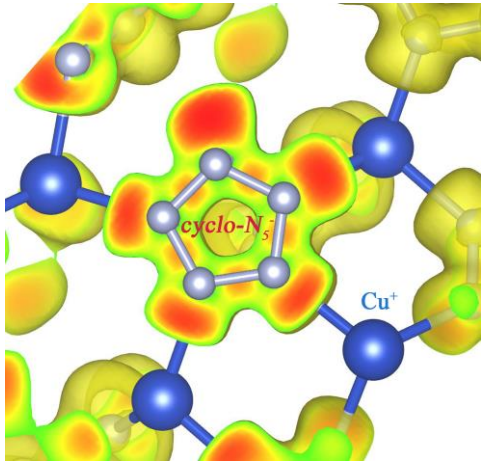
# 含能材料（叠氮化合物）



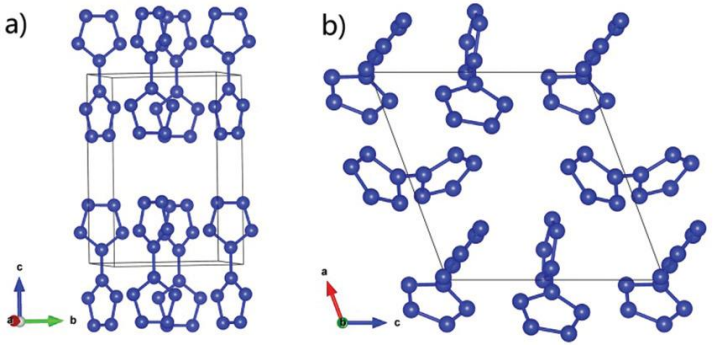

*Mater. Des.* 193 (2020): 108820.




*CrystEngComm* 22.36 (2020): 6057-6062.



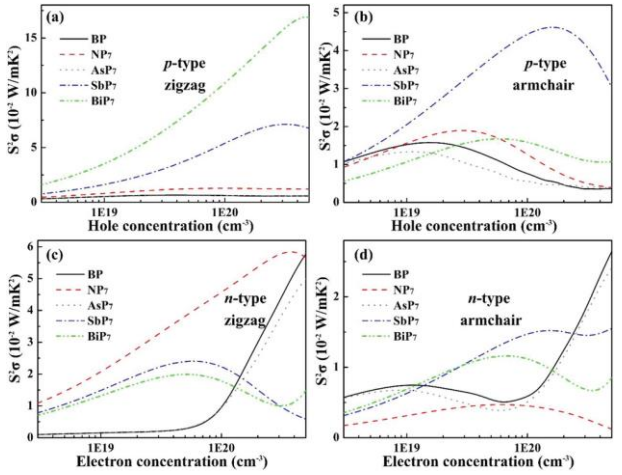

*ACS omega* 5.11 (2020): 6221-6227.



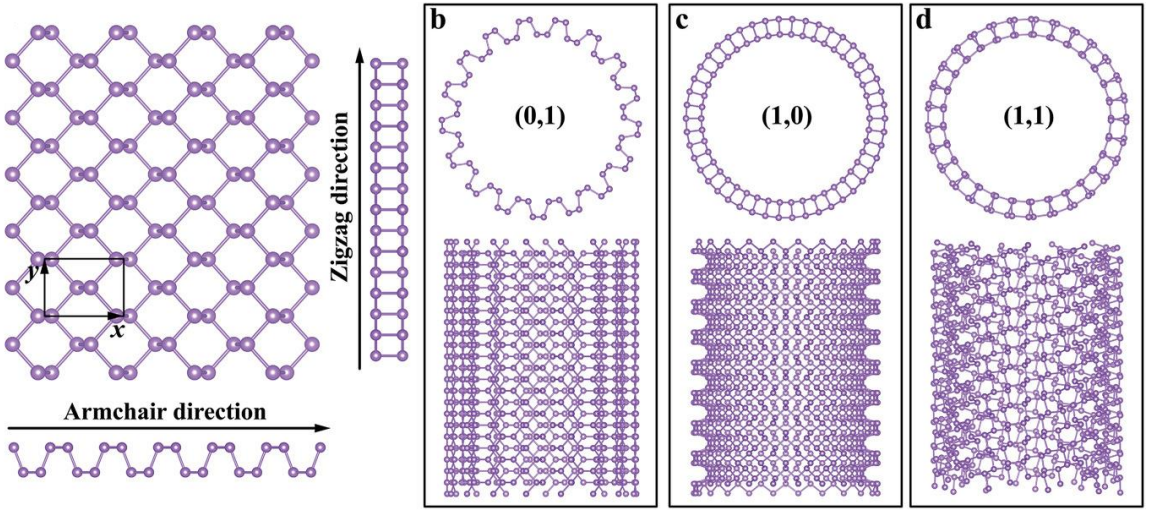

*Adv. Sci.* 7.10 (2020): 1902320.

*核心问题：高稳定性、高含能性、高爆炸冲击性*

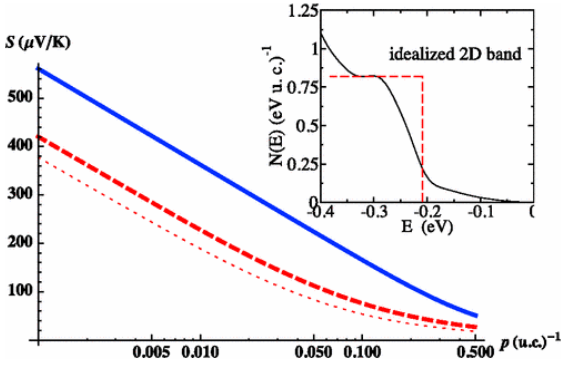
# 热电材料



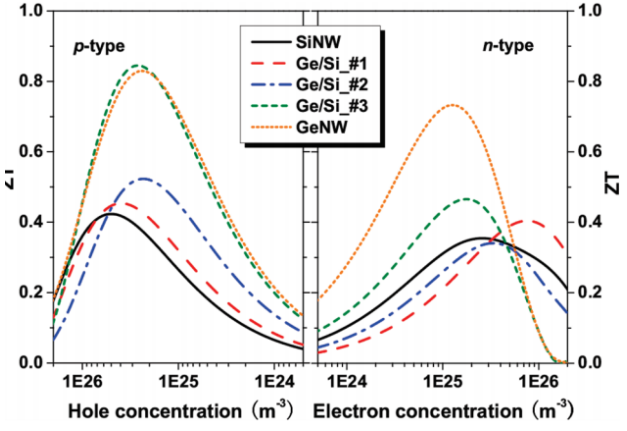

*Adv. Funct. Mater.* 29.38 (2019): 1904346.



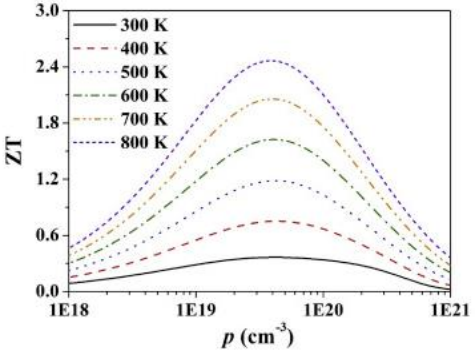

Small, 16, 28 (2020), 2001820




*Phys. Rev. Lett.* 110.14 (2013): 146601




*J. Phys. Chem. C* 114.19 (2010): 9096-9100

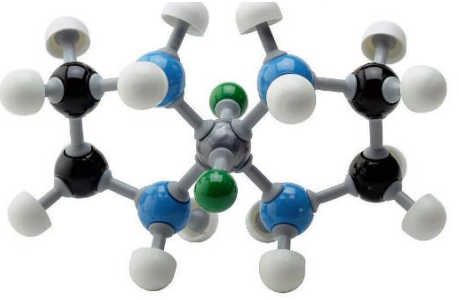



*Vacuum* 170 (2019): 108964.

*核心问题：降低热导率、提高电导率、无毒*

# 密度泛函理论的应用领域

- 随着密度泛函理论的发展，它的应用领域越来越广泛，在物理、化学和生物等多门学科中，密度泛函理论已成为强有力的研究工具。
- 密度泛函理论研究涉及的体系



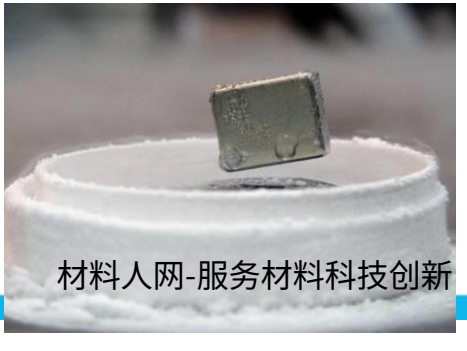
✓零维（如小分子、团簇、量子点）

✓一维（如纳米管）

✓二维（如固体表面、二维材料）

✓三维（如高温超导）

具备功能导向性的材料



# 计算模拟体系

**几何性质**
结构参数（键长、键角、晶格参数、原子位置），稳定构型等
**电子性质**
电子态密度，能带结构，电荷密度分布，电子局域化函数（ELF）等
**状态方程和力学性质**
体弹性模量和弹性常数等
**表面性质**
表面重构、缺陷等结构，表面能量，STM模拟，表面吸附能，反应机理等

光学性质
介电常数，吸收光谱，折射率等
分子动力学模拟
扩散系数和粘性系数
磁学性质
共线和非共线性磁性
自旋轨道耦合
晶格动力学性质
声子谱等
计算材料的激发态（GW准粒子修正）

物理：声, 光, 热, 力, 电
化学：吸附能力、气敏性质、反应焓变、反应能垒
生物：蛋白质折叠、药物设计

# 第一性原理计算常用开源软件对比

| Code Name | Basis Set | Pseudopotential Codes | 操作系统 | Web Site |
|---|---|---|---|---|
| ABINIT | Plane waves | Pseudo, PAW | Linux | www.abinit.org |
| Quantum ESPRESSO | Plane waves | Pseudo | Linux | www.pwscf.org/ |
| CP2K | Mixed gaussian and plane waves | Pseudo or all-electron | Linux | https://www.cp2k.org |
| Exciting | Plane waves | all-electron, full-potential | Linux | http://exciting-code.org |
| Siesta | atomic orbitals | norm-conserving pseudopotentials | Linux | https://departments.icmab.es/leem/siesta/ |
| ELK | Plane waves | all-electron, full-potential, | Linux | http://elk.sourceforge.net |

# 第一性原理计算常用开源软件对比

| Code Name | Basis Set | Pseudopotential Codes | 操作系统 | Web Site |
|---|---|---|---|---|
| Gaussian | Gaussian orbitals | Pseudo | Linux | http://gaussian.com |
| CASTEP | Plane waves | Pseudo | Windows Linux | www.tcm.phy.cam.ac.uk/castep/ |
| VASP | Plane waves | Pseudo, PAW | Linux | cms.mpi.univie.ac.at/vasp |
| WIEN2K | Plane-waves + local orbitals | all-electron, full-potential | Linux | www.wien2k.at |
| FHI-aims | numeric atom-centered orbitals | all-electron, full-potential | Linux | https://aimsclub.fhi-berlin.mpg.de/index.php |
| Pwmat (国内开发) | Plane waves | Pseudo | Linux | http://www.pwmat.com |

# 常用量化软件优缺点对比

VASP：适用于周期性体系的计算，提供源码

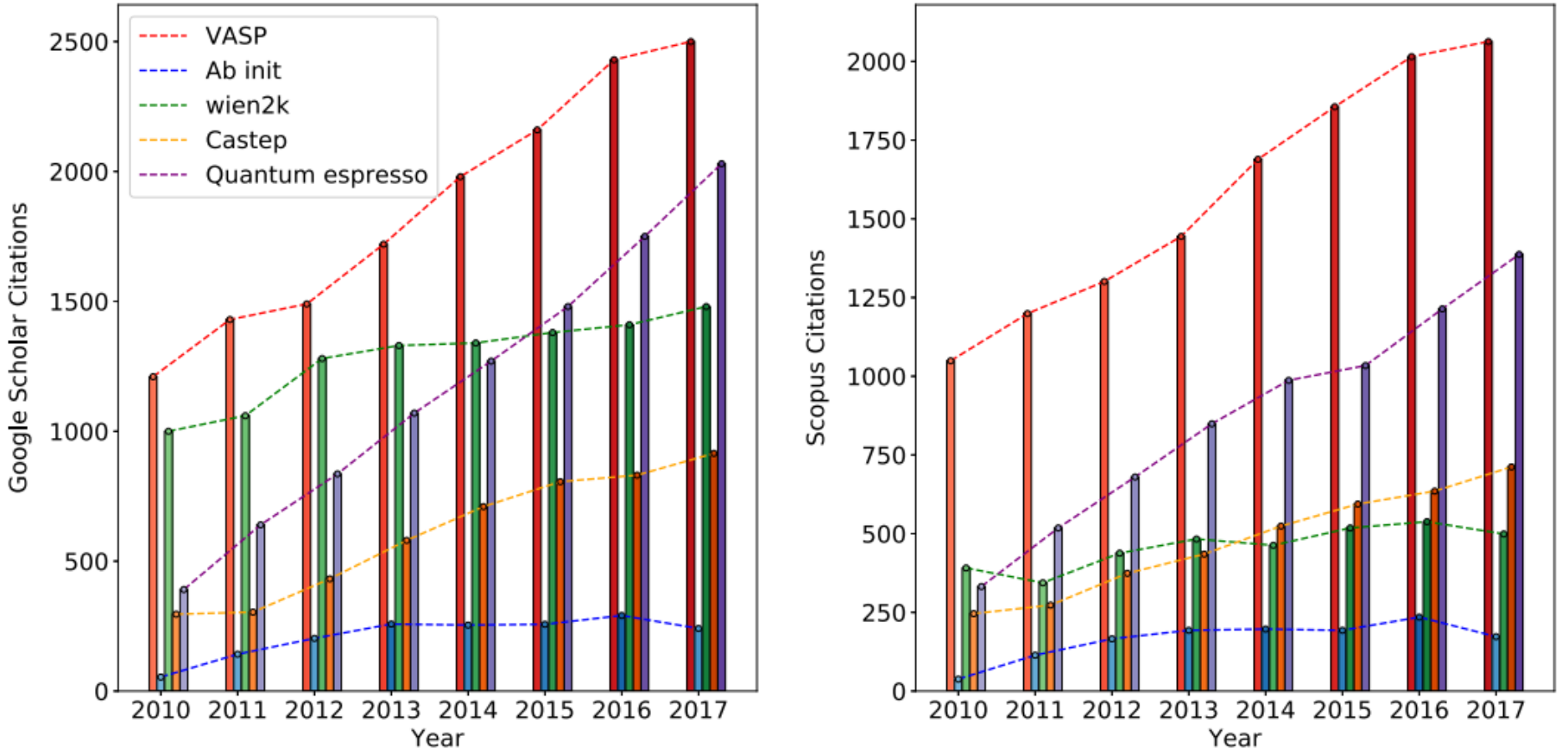
Gaussian：适用于非周期性均相模拟，不提供源码

CASTEP：适用于周期性体系的，提供源码，免费

GROMACS：生物蛋白体系的模拟

其他软件Abinit, Quantum Espresso, CP2K, Lammps, wien2k

# 第一性原理计算常用开源软件对比




Journal of computational chemistry, 2018, 39(26): 2251-2261.

# 第一讲 密度泛函理论及软件简介

易文才

# 主要内容

一、推荐书目

二、VASP理论背景

三、VASP模拟体系

四、VASP的常用工具

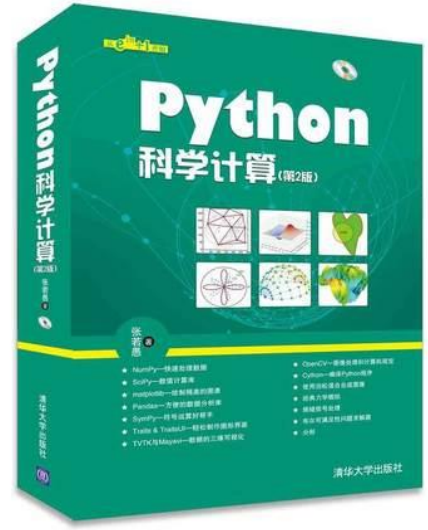

VASP the GUIDE

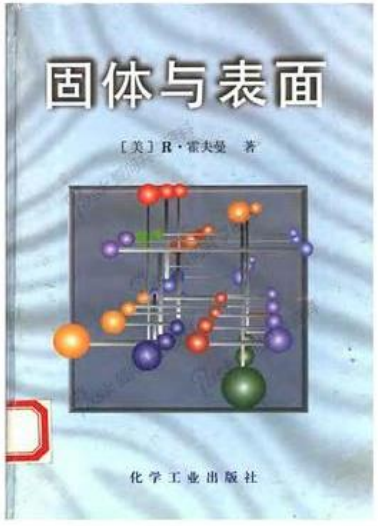
# 一、推荐书目

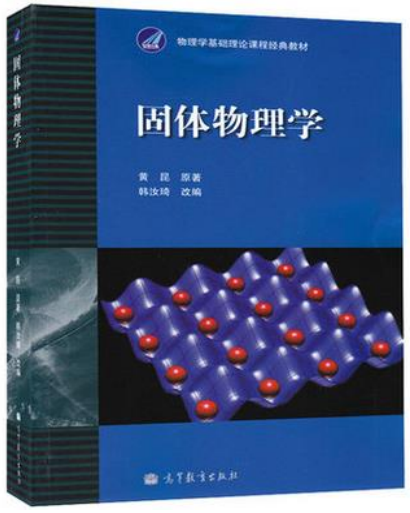
- VASP 官方manual
- 大师兄科研网（http://www.bigbrosci.cn/）
- VASP软件包的使用入门教程　　侯柱峰 2005
- VASP的安装与使用说明　苏长荣 2003
- 精析VASP 太原理工大学 2014

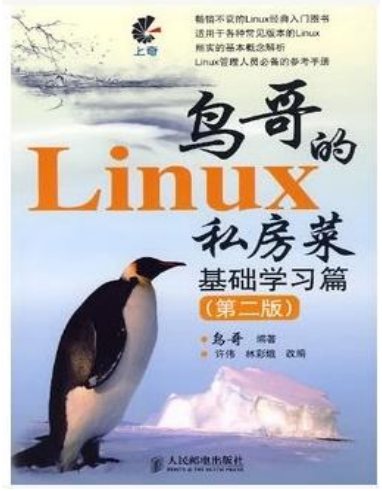
# 一、推荐书目

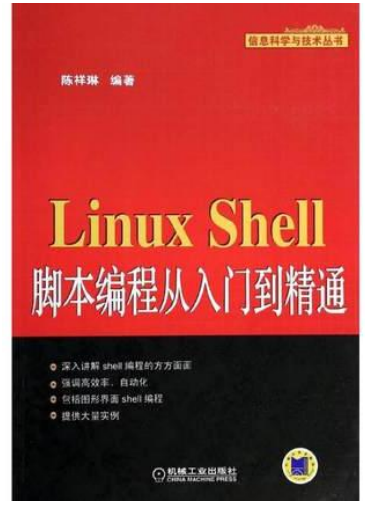
- 《固体物理》 黄昆
- 《固体与表面》霍夫曼
- 《鸟哥的Linux私房菜》 鸟哥 第二版
- 《Fotran 95/2003 程序设计》




# 主要类容

一、推荐书目

二、VASP理论背景

三、VASP模拟体系

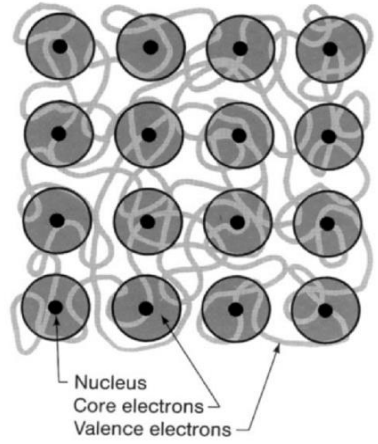
四、VASP的常用工具


VASP the GUIDE

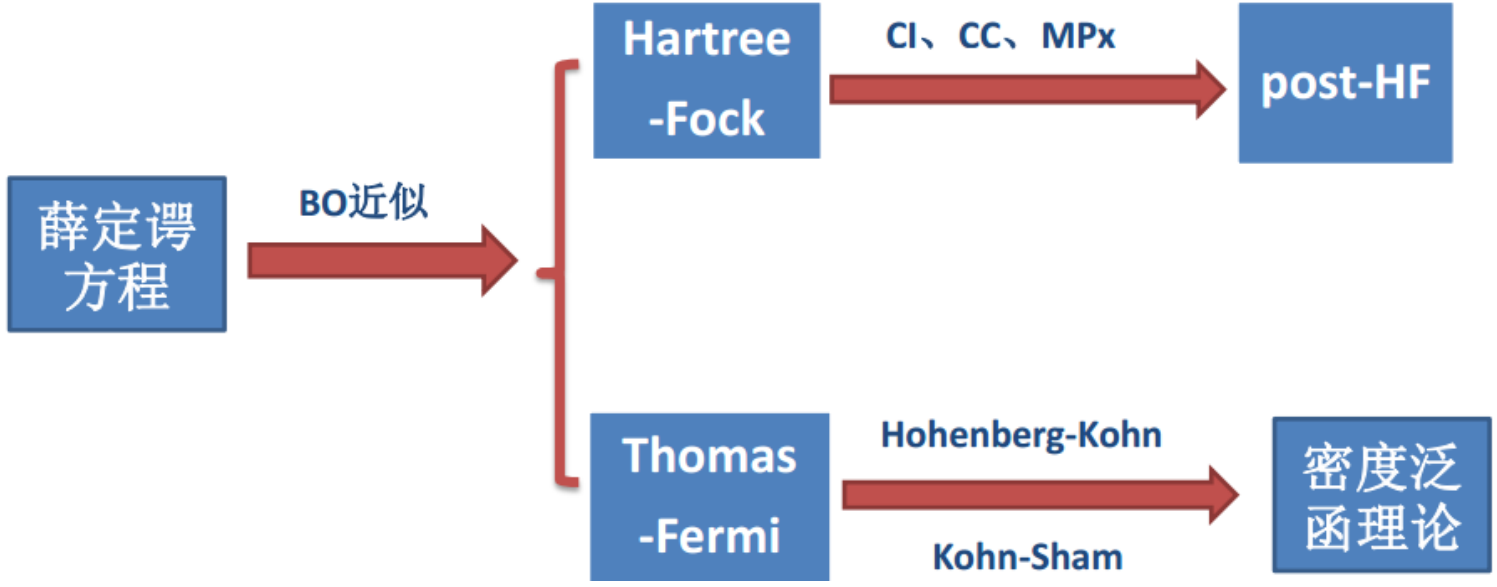
# 二、VASP理论背景

➢薛定谔方程遭遇的困境

仅仅能够精确求解类氢原子体系（H，$H_2^+$,$He^+$）




➢密度泛函理论的形成




核心问题：电子运动方程、核运动方程

# 二、VASP理论背景

## ➢密度泛函理论

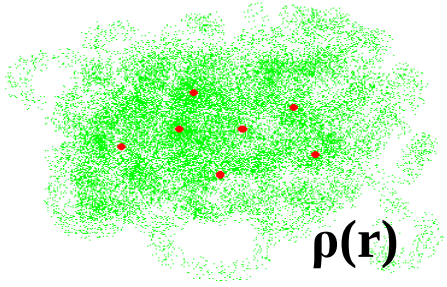
HK 第一定理：证明了体系的基态能量**只与**电荷密度有关，是电荷密度的泛函。

$$E[\rho(\vec{r})] = G[\rho(\vec{r})] + \int V_{ext}(\vec{r})\rho(\vec{r})d^3r + \frac{1}{2}\int\frac{\rho(\vec{r})\rho(\vec{r})}{|\vec{r}-\vec{r}'|}d^3r'd^3r$$

$G[\rho(\vec{r})]$ ： kinetic energy + the rest … the exact form is unknown

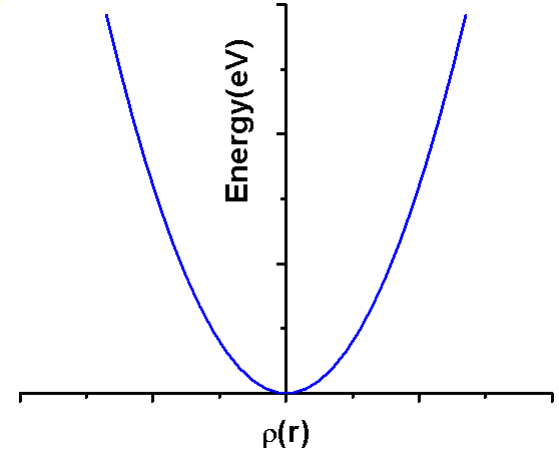
HK 第二定理：证明了以基态密度为变量，将体系能量**最小化**之后就得到了基态能量。

$$\frac{\delta E[\rho(\vec{r})]}{\delta\rho(\vec{r})}\Big|_{\rho_0(\vec{r})} = 0 \quad \text{subject to the condition} \quad \int\delta\rho(\vec{r})d^3r = 0$$




$$E_0 = \min_{\rho\to N} E[\rho]$$

**Total Energy → E[ρ(r)]({R$_i$}$_{i=1,N}$)**



# 二、VASP理论背景

## Kohn-Sham方程

电荷密度分布函数可以写成单电子轨道函数的形式：

$$\rho(\vec{r}) = \sum_i |\phi_i(\vec{r})|^2$$

于是，Kohn-sham等式可以写成：

$$\{-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + \int \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} d^3r' + \mu_{xc}[\rho(\vec{r})]\}\phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r})$$

$$V_{eff}(\vec{r}, \rho(\vec{r}))$$

$$\mu_{xc}[\rho(r)] = \frac{\delta E_{xc}[\rho(\vec{r})]}{\delta \rho(\vec{r})}$$

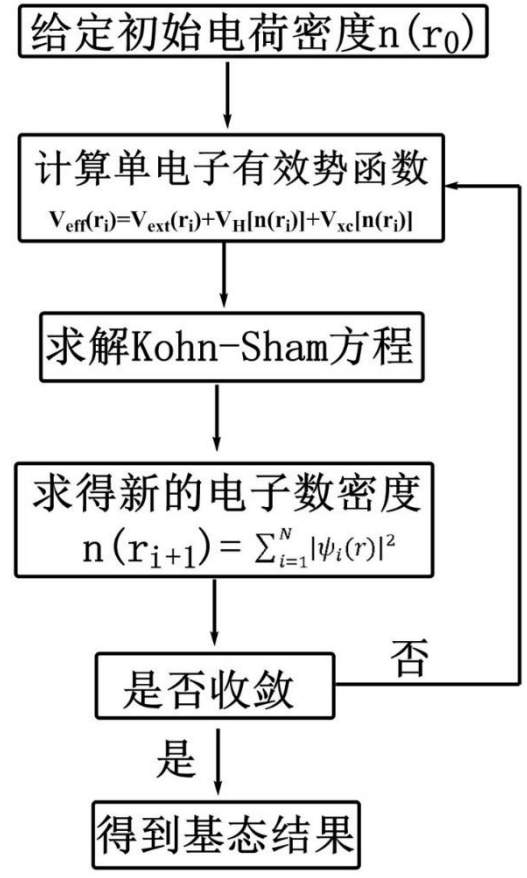
# 二、VASP理论背景

## 求解Kohn-Sham方程

$$\left\{-\frac{\nabla^2}{2}+v_{eff}(\vec{r})\right\}\varphi_{i,s}(\vec{r})=\varepsilon_{i,s}\varphi_{i,s}(\vec{r})$$

$$n(\vec{r})=\sum_{i=1}^{N_s}\sum_{s=1}^{2}\left|\varphi_{i,s}(\vec{r})\right|^2$$

$$v_{eff}(\vec{r})=v(\vec{r})+\int\frac{n(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d\vec{r}'+\mu_{XC}\left[n(\vec{r})\right]$$




**Kohn-sham求解流程图**

**总能：** $$\sum_{i=1}^{N_s}\sum_{s=1}^{2}\varepsilon_{i,s}-\frac{1}{2}\iint\frac{n(\vec{r})n(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|}d\vec{r}d\vec{r}'+\left\{E_{XC}\left[n(\vec{r})\right]-\int n(\vec{r})\mu_{XC}\left[n(\vec{r})\right]d\vec{r}\right\}$$

# 二、VASP理论背景

| | N | E | dE | d eps | ncg | rms | rms(c) |
|---|---|---|---|---|---|---|---|
| DAV: | 1 | 0.633507539466E+03 | 0.63351E+03 | -0.11227E+04 | 256 | 0.467E+02 | |
| DAV: | 2 | 0.227367978092E+03 | -0.40614E+03 | -0.36313E+03 | 480 | 0.707E+01 | |
| DAV: | 3 | 0.239901003533E+01 | -0.22497E+03 | -0.21432E+03 | 416 | 0.965E+01 | |
| DAV: | 4 | -0.199630275759E+02 | -0.22362E+02 | -0.21624E+02 | 384 | 0.473E+01 | |
| DAV: | 5 | -0.204255083389E+02 | -0.46248E+00 | -0.46009E+00 | 336 | 0.708E+00 | 0.149E+01 |
| DAV: | 6 | -0.220476431435E+02 | -0.16221E+01 | -0.11944E+02 | 368 | 0.390E+01 | 0.213E+01 |
| DAV: | 7 | -0.156975580063E+02 | 0.63501E+01 | -0.11411E+02 | 416 | 0.319E+01 | 0.107E+01 |
| DAV: | 8 | -0.160403999422E+02 | -0.34284E+00 | -0.32595E+01 | 416 | 0.226E+01 | 0.118E+01 |
| DAV: | 9 | -0.143135529476E+02 | 0.17268E+01 | -0.23075E+01 | 432 | 0.147E+01 | 0.780E+00 |
| DAV: | 10 | -0.133359637804E+02 | 0.97759E+00 | -0.26576E+00 | 368 | 0.849E+00 | 0.493E+00 |
| DAV: | 11 | -0.139894790060E+02 | -0.65352E+00 | -0.42245E-01 | 352 | 0.284E+00 | 0.346E+00 |
| DAV: | 12 | -0.149434700784E+02 | -0.95399E+00 | -0.90936E-01 | 368 | 0.350E+00 | 0.196E+00 |
| DAV: | 13 | -0.153584661579E+02 | -0.41500E+00 | -0.23016E-01 | 320 | 0.245E+00 | 0.148E+00 |
| DAV: | 14 | -0.156344341255E+02 | -0.27597E+00 | -0.13501E-01 | 384 | 0.220E+00 | 0.114E+00 |
| DAV: | 15 | -0.158720908747E+02 | -0.23766E+00 | -0.63952E-02 | 288 | 0.136E+00 | 0.586E-01 |
| DAV: | 16 | -0.160325017447E+02 | -0.16041E+00 | -0.44718E-02 | 336 | 0.860E-01 | 0.455E-01 |
| DAV: | 17 | -0.160937189664E+02 | -0.61217E-01 | -0.99653E-03 | 368 | 0.603E-01 | 0.278E-01 |
| DAV: | 18 | -0.161932531329E+02 | -0.99534E-01 | -0.13324E-02 | 288 | 0.461E-01 | 0.212E-01 |
| DAV: | 19 | -0.162571479941E+02 | -0.63895E-01 | -0.55004E-03 | 336 | 0.315E-01 | 0.112E-01 |
| DAV: | 20 | -0.163107072796E+02 | -0.53559E-01 | -0.39243E-03 | 304 | 0.191E-01 | 0.895E-02 |
| DAV: | 21 | -0.163502223175E+02 | -0.39515E-01 | -0.33566E-03 | 288 | 0.169E-01 | 0.479E-02 |
| DAV: | 22 | -0.163672903326E+02 | -0.17068E-01 | -0.14301E-03 | 256 | 0.104E-01 | 0.339E-02 |
| DAV: | 23 | -0.163747564736E+02 | -0.74661E-02 | -0.58517E-04 | 288 | 0.697E-02 | 0.226E-02 |
| DAV: | 24 | -0.163804189220E+02 | -0.56624E-02 | -0.53200E-04 | 272 | 0.623E-02 | 0.161E-02 |
| DAV: | 25 | -0.163818776539E+02 | -0.14587E-02 | -0.26830E-04 | 240 | 0.459E-02 | 0.921E-03 |
| DAV: | 26 | -0.163825677332E+02 | -0.69008E-03 | -0.14032E-04 | 256 | 0.317E-02 | 0.630E-03 |
| DAV: | 27 | -0.163835388301E+02 | -0.97110E-03 | -0.73362E-05 | 224 | 0.274E-02 | 0.836E-03 |
| DAV: | 28 | -0.163841910815E+02 | -0.65225E-03 | -0.46717E-05 | 240 | 0.191E-02 | 0.506E-03 |
| DAV: | 29 | -0.163846551817E+02 | -0.46410E-03 | -0.30634E-05 | 240 | 0.139E-02 | 0.316E-03 |

能量本正值：能带结构、态密度

波函数：电荷密度、电荷信息

自旋：磁矩、自旋电荷密度等

能量信息：吸附能、力学性质、频率、反应能垒等

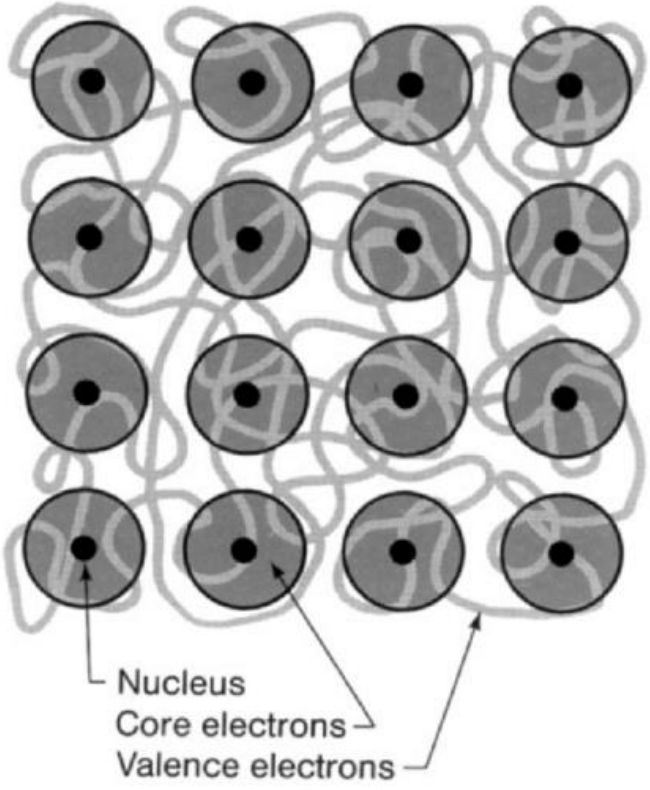
**VASP输出文件OSZICAR文件**

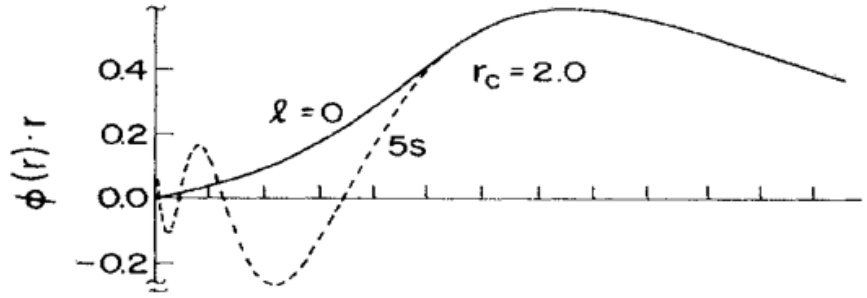
简单：所有的求解过程，已经封装到VASP程序包中，对大部分用户而言，仅仅学习输入文件编写，即可完成材料计算模拟。

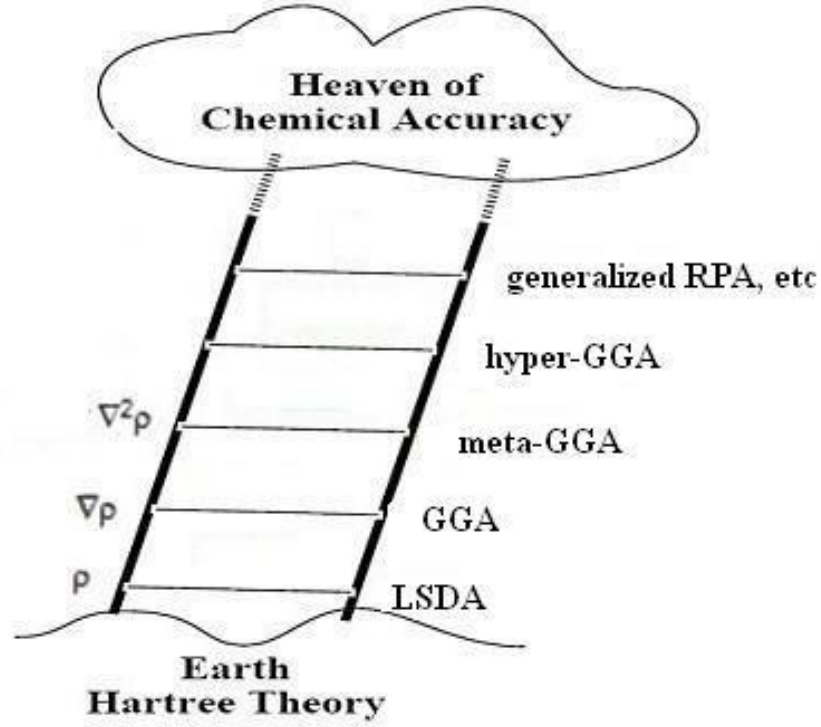
不简单：用户需了解每个参数背后的物理意义，不然就真成暗箱操作了

# 二、VASP理论背景

## 赝势方法




总能没有意义，差值才有意义

**雅各布天梯**

# 二、VASP理论背景

## 本章小结

- 从薛定谔方程到密度泛函理论的发展历史
- Kohn-sham方程：一个自洽迭代方程组，能够通过自洽迭代迅速地求解一个体系的电荷密度分布函数$\rho(\vec{r})$，从而解决多电子体系薛定谔方程求解困难的窘境。
- 赝势：通过一个假想的势能函数替代内层电子波函数震荡的情形，从而大大减小计算量的方法。

# 主要类容

一、推荐书目

二、VASP理论背景

三、VASP模拟体系

四、VASP的常用工具


VASP the GUIDE

# 三、VASP模拟体系

## 适用计算体系（周期性体系）

- 按照维度划分：零维团簇、一维纳米带、二维材料和表面、三维晶体
- 按照计算性质划分：光、电、磁、热
- 按照材料功能划分：能源存储与转化、催化材料、电子功能器件、气敏材料以及高压物理等等

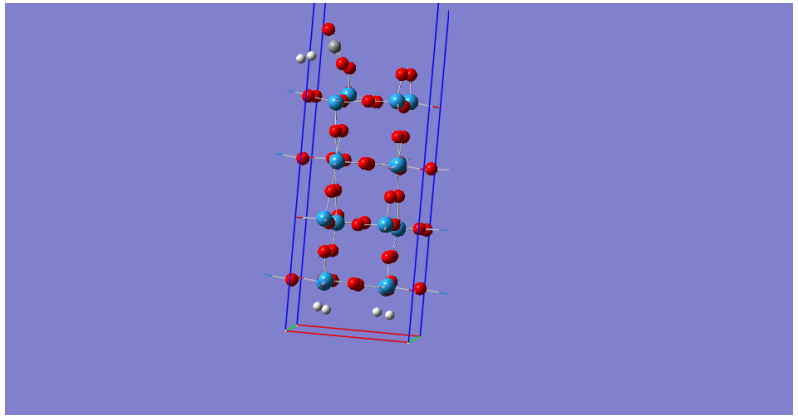
# 三、VASP模拟体系

## 计算范围

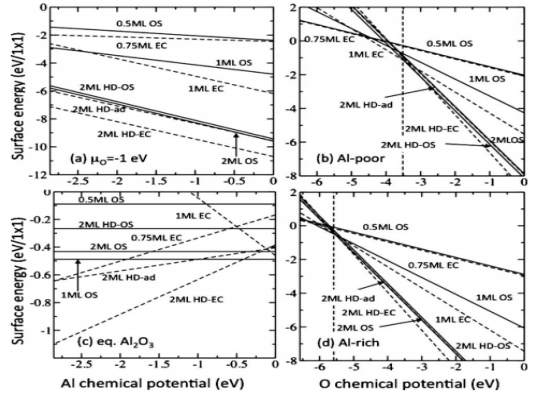
**几何性质**
结构参数（键长、键角、晶格参数、原子位置），稳定构型等
**电子性质**
电子态密度，能带结构，电荷密度分布，电子局域化函数（ELF）等
**状态方程和力学性质**
体弹性模量和弹性常数等
**表面性质**
表面重构、缺陷等结构，表面能量，STM模拟，表面吸附能，反应机理等

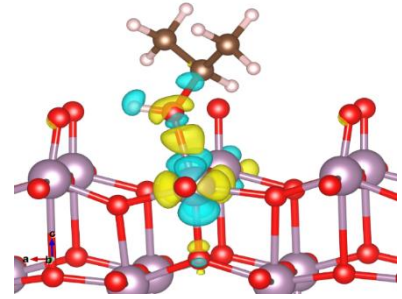
**光学性质**
介电常数，吸收光谱，折射率等
**分子动力学模拟**
扩散系数和粘性系数
**磁学性质**
共线和非共线性磁性
自旋轨道耦合
**晶格动力学性质**
声子谱等
**计算材料的激发态（GW准粒子修正）**

# 三、VASP模拟体系

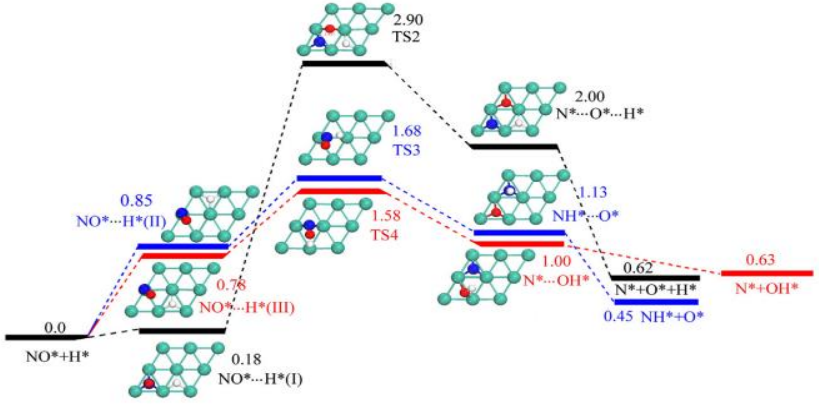


1）几何优化

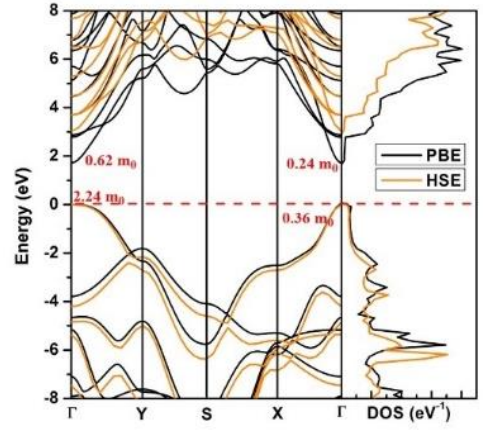


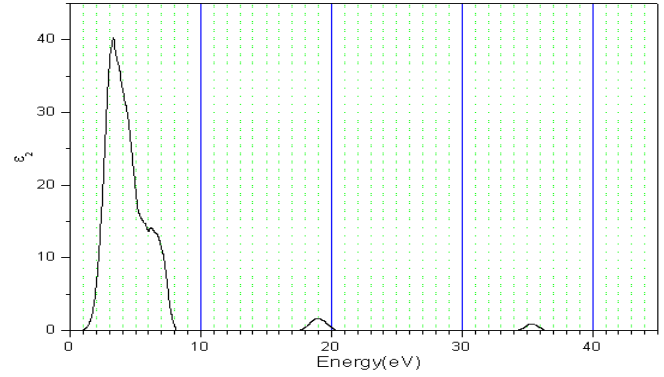
2）能量计算：形成能和吸附能




3）过渡态搜索及反应机理计算




4）电子结构




5）介电常数，吸收光谱等

# 三、VASP模拟体系

## 本章小结

- 适用体系：周期性具有重复单元的体系
- 计算功能：固体表面催化反应机理，材料性质计算
- 发展趋势：与实验现象相辅相成，总结规律，预测新物质性质
- 热点关键词：单原子催化，材料基因计划，热电材料，能源材料，电子器件

# 主要类容

一、推荐书目

二、VASP理论背景

三、VASP模拟体系

四、VASP的常用工具


VASP the GUIDE

# 三、VASP的常用工具

## 软件列表

**For Linux**

- qvasp
- vaspkit
- vtstscripts
- p4vasp

**xshell**

**xftp**

**For Windows**

- VESTA
- Origin
- ChemDraw
- Photoshop

# 计算流程

## 输入文件

$a=2$

$b=3$

自己在服务器创建

## 做计算

$c=a+b$


计算程序执行

## 输出文件

$c=5$

计算程序输出，写文件

# qvasp功能

```
+=============================================================================================+
|                                        qvasp usage v2.21                                    |
|                                                    --Written by Wencai,Yi                   |
|                                                         2020.07.18                          |
+=================== POSCAR ================== + =============== POTCAR ======================+
| qvasp -fix  Fix atoms for POSCAR from *.vasp  | qvasp -pw91 ELE_Name  POTCAR from PW91        |
| qvasp -t    Insert points for TS cal.(method1)| qvasp -pbe ELE_Name   POTCAR from PBE         |
| qvasp -t2   Insert points for TS cal.(method2)| qvasp -lda ELE_Name   POTCAR from LDA         |
| qvasp -sc   Create supercell for POSCAR       | qvasp -cp             Check the POTCAR        |
| qvasp -zc   Correct imaginary frequency      +================== KPOINTS ====================+
| qvasp -c2p  Transfer cif file to POSCAR       | qvasp -k number    Create KPOINTS(Auto mesh)  |
+=================== INCAR ================== + ================== Tools ====================+
| qvasp -relax   For Structure Optimization cal.| qvasp -gauss      Transfer OUTCAR to Gauss log |
| qvasp -ts      For Trasition State cal.       | qvasp -e          Read energy from OUTCAR      |
| qvasp -scf     For Self_Consistent cal.       | qvasp -p2c        Transfer format to *.cif     |
| qvasp -elf     For Eelectron Local Function   | qvasp -findcell   Find the pri-cell of CONTCAR |
| qvasp -wk      For Work Fuction cal.          | qvasp -wkd        Get Work Function from LOCPOT|
| qvasp -band    For Energy Band cal.           | qvasp -bandd      Deal Bands data from EIGENVAL|
| qvasp -dos     For Density Of States cal.     | qvasp -dosd       Deal DOS data from DOSCAR    |
| qvasp -bader   For Bader Charge cal.          | qvasp -ldos 1 2   Get LDOS data from DOS1 DOS2.|
| qvasp -hse     For HSE06 cal.                 | qvasp -mde        Read Energy data for AIMD    |
| qvasp -md      For Ab Init Molecular Dynamics | qvasp -mdm        Read Magnetic moment for AIMD|
| qvasp -elastic For Elastic Constants cal.     | qvasp -elasticd   Read elastic constants       |
| qvasp -partchg For PARTICAL Charge cal.       | qvasp -findsym    Find the symmetry            |
| qvasp -freq    For Frequency cal.             | qvasp -zpe        Get ZPE value                |
| qvasp -optics  For Optics Property cal.       | qvasp -opticsd    Get optics datas             |
| qvasp -phono   For Phonon Spectrum cal.       | qvasp -3dband     Get 3D band for 2D materials |
+================================== Customizable Tools =======================================+
| qvasp -nanotube POSCAR           Rolling nanosheet to POSCAR-nanotube                       |
| qvasp -out2arc                   Get trajectory file from OUTCAR to arc(opened by MS)       |
| qvasp -cleavesurface POSCAR      Cleave surface from POSCAR                                 |
| qvasp -heterojunction str1 str2  Construct heterojunction str1 and str2(python3)(JunLuo etc.)  |
| qvasp -vaspkit                   Call VASPKIT program,ref:arXiv preprint arXiv:1908.08269   |
| qvasp -baderd                    Obtian bader charge information                            |
| qvasp -3dkpoints                 Produce KPOINTS for 3D band for 2D materisl (-0.5 to 0.5)  |
| qvasp -clean                     Clear all file except POSCAR INCAR KPOINTS POTCAR          |
+================================== Devoloper Info ===========================================+
| Cite with "The calculations were assisted by the qvasp code [1]"      QQ Group: 398274903   |
| [1] W. Yi, G. Tang, et al.qvasp: A Flexible Toolkit for VASP Users in Materials Simulations |
+=============================================================================================+
```

# 实例演示

如何登录服务器？
如何创建输入文件？
如何提交计算任务？

**请各位提前熟悉Linux基本命令：**
**cd; ls; mkdir; rm; mv; cp; vi; 环境变量概念**

# 第二讲 VASP的主要输入和输出

易文才

# 主要内容

一、VASP的四个输入文件

二、VASP的输出文件

三、与VASP相关搭配软件的使用

四、Linux下常用配套命令


VASP the GUIDE

# 一、VASP的四个输入文件

文件名必需大写

INCAR : 其内容为关键词，确定了计算参数以及目的；

POSCAR : 结构描述文件，主要包括平移矢量、原子类型和数目、以及各原子坐标；

KPOINTS : K点定义文件，三种模式；

POTCAR : 原子的赝势文件；

思考：这四个文件缺一不可吗？

答案：5.2.12 KPOINTS文件不再必须，但建议设置

# 一、VASP的四个输入文件

**INCAR控制算法**

(1)电子算法控制参数

PREC、ALGO、ENCUT、EDIFF、NELM、ISPIN、GGA、VOSKOWN、MAGMOM、NUPDOWN、ISMEAR等

(2) 粒子算法控制参数

IBRION、POTIM、NSW、EDIFFG、ISIF等

(3) 输出控制参数

LCHARG、LWAVE、LORBIT、LELF、LVTOT等

(4) 其他控制参数

SYSTEM 、NPAR等

Ref: http://cms.mpi.univie.ac.at/vasp/vasp/Index.html

```
SYSTEM =  AlN 0001 surface 2x2 Ga_T4

Electronic strcutre
  PREC    = normal
  ENCUT   = 400 eV ; NELMIN = 2 ; NELMDL = -5
  EDIFF   = 1E-5
  EDIFFG = -0.01
  LREAL   = Auto    real space projections

  LCHARG = .FALSE.
  LWAVE   =  F

  GGA = PE

Ionic Relaxation
  NSW     = 300     number of steps for IOM
  IBRION = 2
  ISIF    = 3

DOS related values:
  ISMEAR =     0  ; SIGMA = 0.01
```

INCAR关键词(部分参考清华大学物理系苏长荣编写的VASP安装和使用说明)

# INCAR常见设置

## LDA+U:

LDAU=.TRUE.  ## For LDA + U set
LDAUTYPE=2
LDAUL= 3 -1
LDAUU=5.0  0
LDAUJ= 0  0

## 磁性：

ISPIN=2
MAGMOM=-4 4.0 4*0

## 范德华力一：

IVDW=11

## 溶剂化效应：

LSOL=TRUE
EB_k = 60

问题来了：易老师能记住这些设置吗？

## HSE06:

LHFCALC  = .TRUE.
ISTART = 1
HFSCREEN  = 0.2
ICHARG = 2
AEXX = 0.25
ALGO = Damped
Time = 0.4
PRECFOCK  = N

```
TiO2_anatase
   1.00000000000000
     5.5105964896540316    0.0072576945966098   -0.0000857011140024
     2.8646258590377451    4.7077059373335759   -0.0000856330136410
    -4.1876516303982578   -2.3575045513242316    2.6970952011585361
   Ti   O
     2     4
Direct
 -0.0000004161018627 -0.0000000526922796 -0.0000003634095822
  0.7500004161018627  0.2500000526922795  0.5000003634095822
```

## 范德华力二（需放vdw_kernel.bindat）：

GGA = BO
PARAM1 = 0.1833333333
PARAM2 = 0.2200000000
LUSE_VDW = .TRUE.
AGGAC = 0.0000

## 自旋轨道耦合：

LSORBIT = .TRUE.

# INCAR模板的产生

```
+=============================================================================================+
|                                      qvasp usage v2.21                                      |
|                                                  --Written by Wencai,Yi                     |
|                                                       2020.07.18                            |
+=================== POSCAR ================== + =============== POTCAR ======================+
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| qvasp -t2   Insert points for TS cal.(method2)| qvasp -lda ELE_Name   POTCAR from LDA         |
| qvasp -sc   Create supercell for POSCAR       | qvasp -cp             Check the POTCAR        |
| qvasp -zc   Correct imaginary frequency      +================== KPOINTS ====================+
| qvasp -c2p  Transfer cif file to POSCAR       | qvasp -k number    Create KPOINTS(Auto mesh)   |
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 qvasp -wk      For Work Fuction cal.            qvasp -wkd        Get Work Function from LOCPOT|
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 qvasp -partchg For PARTICAL Charge cal.         qvasp -findsym    Find the symmetry            |
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| [1] W. Yi, G. Tang, et al.qvasp: A Flexible Toolkit for VASP Users in Materials Simulations |
+=============================================================================================+
```

# 一、VASP的四个输入文件

## POSCAR文件

AlN bulk (Title)

1.0 (Scaling factor or lattice constant)

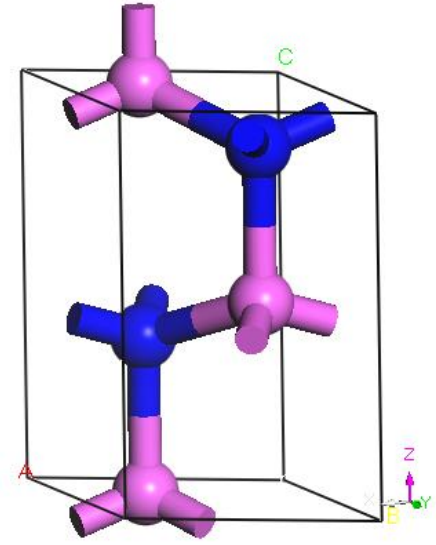
3.11 0.00 0.00(第一个平移矢量的方向)

-1.56 2.69 0.00 (第二个平移矢量的方向)

0.00 0.00 4.98 (第三个平移矢量的方向)

Al N

2 2 (单胞内原子数目以及原子种类)




Selective dynamics(表示对构型进行部分优化，如果没这行，则表示全优化)

Direct (表示所采用的为分数坐标，如果内容为Car，则坐标单位为埃)

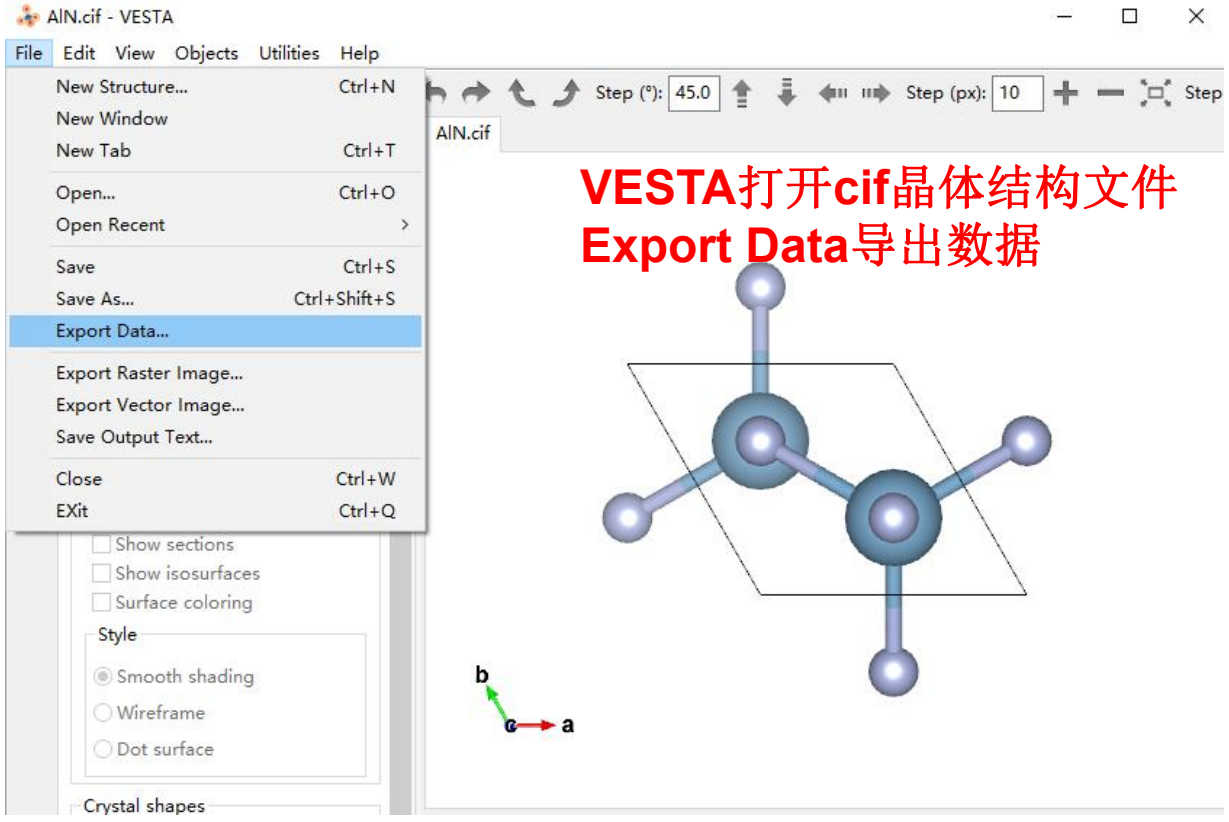
0.667 0.333 0.000 T T T (各原子坐标以及哪个方向坐标放开优化)

0.333 0.667 0.500 T T T

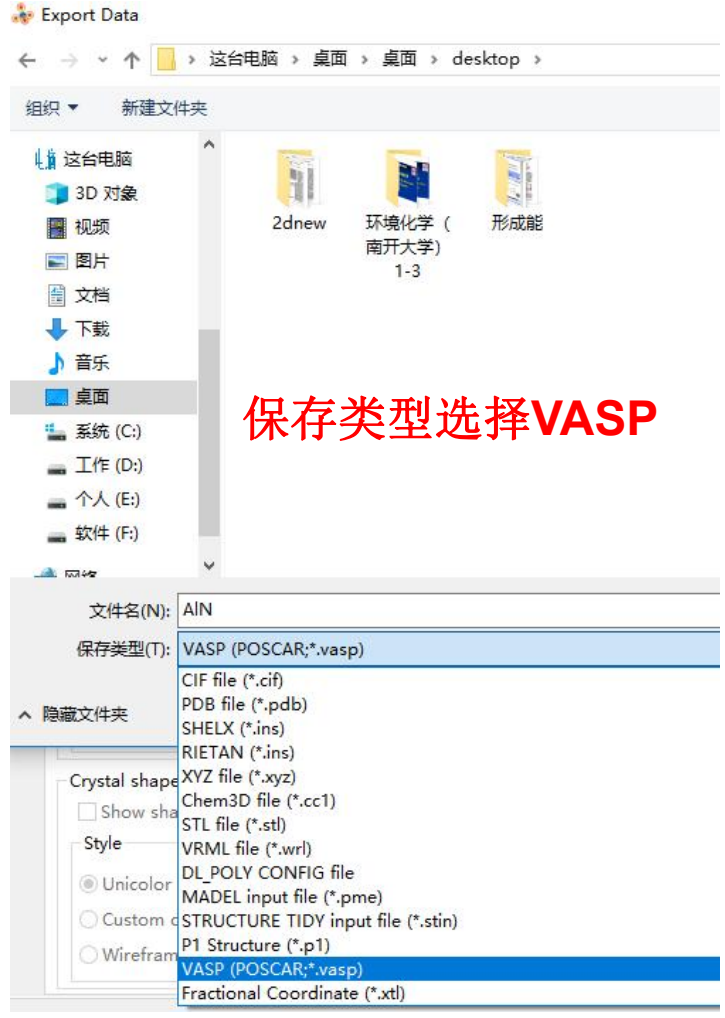
0.667 0.333 0.382 T T T

0.333 0.667 0.882 F F F

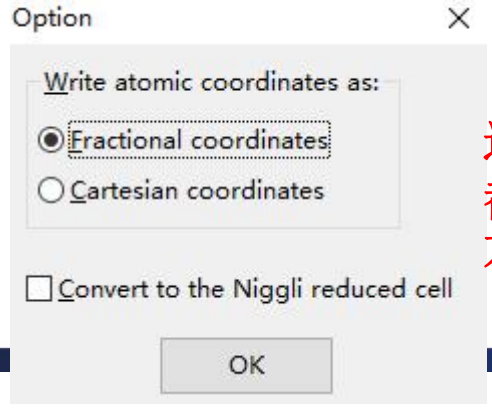
# POSCAR产生




**VESTA打开cif晶体结构文件**
**Export Data导出数据**




**保存类型选择VASP**




**选择分数坐标和笛卡尔坐标**
**都可以**
**不必勾选转化成原胞，除非你想这样**

**也可以选择用qvasp –c2p的工具来直接转化cif文件成POSCAR**

# 一、VASP的四个输入文件

KPOINTS文件

一般有三种定义K点的方法：

1) 通过定义K-mesh大小，由程序自动产生各K点：

Automatic mesh (title)

0 (为0时，表示自动产生K点)

M (表示采用Monkhorst-Pack方法生成K点坐标)

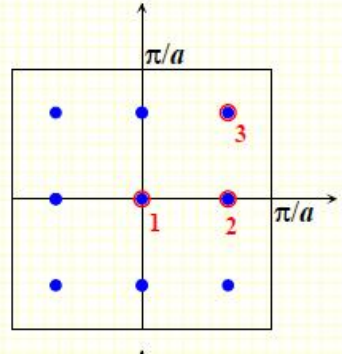
K1 K2 K3(对应于K1 x K2 x K3网格，K-mesh)

0 0 0(原点平移大小)

Examples

- $N_1$=$N_2$=3 total 9 k points
- including Γ point
- 3 irreducible points
- weighting factors

$\alpha_1 = 1/9, \alpha_2 = 4/9, \alpha_3 = 4/9$




Our first-principles calculations were based on the density functional theory within the PBE approximation for the exchange–correlation energy.[41–43] The core–valence interactions were described by the projector augmented-wave (PAW) potentials,[44] as implemented in the VASP code. Plane waves with a kinetic energy cutoff of 600 eV were used as the basis set. The calculations were carried out in periodic super cells. The atomic positions were optimized by using the conjugate gradient method, in which the energy convergence criterion between two consecutive steps was set at $10^{-5}$ eV. The maximum allowed force on the atoms is $10^{-2}$ eV $Å^{-1}$. The *k*-point meshes 7 × 7 × 13 and 5 × 5 × 13 were used for the Brillion Zone (BZ) integration of CHC-1 and CHC-2, respectively.[45] When calculating the adsorption of gaseous atoms/molecules, the Grimme-D3 correction was included in the calculation to account for van der Waals interactions.[46,47] Phonon spectra were obtained by using the Phonopy package.[48]

# 一、VASP的四个输入文件

## 如何定义K点网格？

AlN bulk (Title)

1.0 (Scaling factor or lattice constant)

3.11 0.00 0.00(第一个平移矢量的方向)

-1.56 2.69 0.00 (第二个平移矢量的方向)

0.00 0.00 4.98 (第三个平移矢量的方向)

Al N

2 2 (单胞内原子数目以及原子种类)

Selective dynamics(表示对构型进行部分优化，如果没这行，则表示全优化)

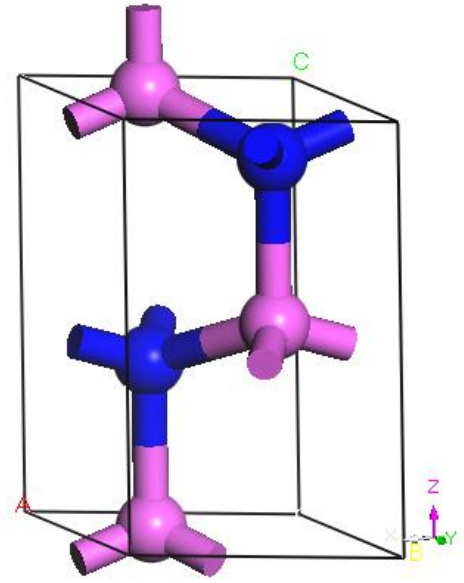
Direct (表示所采用的为分数坐标，如果内容为Car，则坐标单位为埃)

0.667 0.333 0.000 T T T (各原子坐标以及哪个方向坐标放开优化)

0.333 0.667 0.500 T T T

0.667 0.333 0.382 T T T

0.333 0.667 0.882 F F F




KPOINTS：

Auto

0

G

5 5 3

0. 0. 0.

六方晶系需取G

真空方向设为1

方法一

*a*=3.11； *b*=3.11； *c*=4.98

*a**K1=*b**K2=*c**K3

K1=5 K2=5 K3=3

K-mesh： 5 5 3

方法二

*a*=3.11； *b*=3.11； *c*=4.98

K1=INIT(2*π/*a*/0.4)=5

K2=INIT(2*π/*b*/0.4)=5

K3=INIT(2*π/*c*/0.4)=3

# 自动网格KPOINTS产生器

```
+=============================================================================================+
|                                        qvasp usage v2.21                                    |
|                                                  --Written by Wencai,Yi                     |
|                                                       2020.07.18                            |
+=================== POSCAR ================== + ================ POTCAR ======================+
| qvasp -fix  Fix atoms for POSCAR from *.vasp  | qvasp -pw91 ELE_Name  POTCAR from PW91        |
| qvasp -t    Insert points for TS cal.(method1)| qvasp -pbe ELE_Name   POTCAR from PBE         |
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| qvasp -zc   Correct imaginary frequency       +================== KPOINTS ====================+
| qvasp -c2p  Transfer cif file to POSCAR       | qvasp -k number    Create KPOINTS(Auto mesh)  |
+=================== INCAR =================== + ================== Tools ======================+
| qvasp -relax   For Structure Optimization cal.| qvasp -gauss      Transfer OUTCAR to Gauss log |
| qvasp -ts      For Trasition State cal.       | qvasp -e          Read energy from OUTCAR      |
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| qvasp -elf     For Eelectron Local Function   | qvasp -findcell   Find the pri-cell of CONTCAR |
| qvasp -wk      For Work Fuction cal.          | qvasp -wkd        Get Work Function from LOCPOT|
| qvasp -band    For Energy Band cal.           | qvasp -bandd      Deal Bands data from EIGENVAL|
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| qvasp -elastic For Elastic Constants cal.     | qvasp -elasticd   Read elastic constants       |
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| qvasp -heterojunction str1 str2  Construct heterojunction str1 and str2(python3)(JunLuo etc.)|
| qvasp -vaspkit                   Call VASPKIT program,ref:arXiv preprint arXiv:1908.08269   |
| qvasp -baderd                    Obtian bader charge information                            |
| qvasp -3dkpoints                 Produce KPOINTS for 3D band for 2D materisl (-0.5 to 0.5)  |
| qvasp -clean                     Clear all file except POSCAR INCAR KPOINTS POTCAR          |
+================================== Devoloper Info ===========================================+
| Cite with "The calculations were assisted by the qvasp code [1]"      QQ Group: 398274903   |
| [1] W. Yi, G. Tang, et al.qvasp: A Flexible Toolkit for VASP Users in Materials Simulations |
+=============================================================================================+
```

number默认值0.03

qvasp -k能自动识别晶体维度，并设置K点网格，后面跟的数越小，网格越密，K1K2K3越大。

# 一、VASP的四个输入文件

## KPOINTS文件

2) Line-mode (一般仅在计算能带结构时使用)：

k-points for MgO(100) (title)
21 (K点数目)
Line-mode
Rec (字母R打头表示为倒易空间坐标，否则为实空间的坐标)

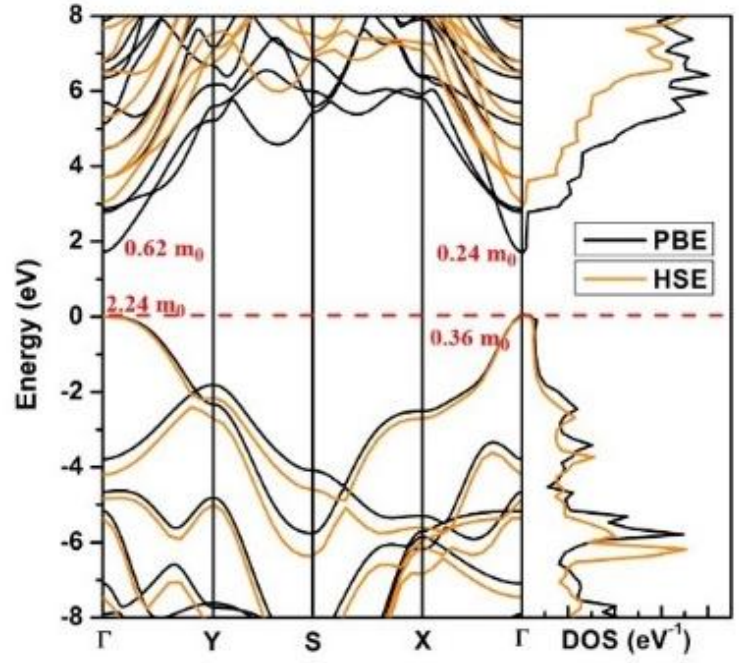
```
0.0  0.0  0.0   ! Γ (各K点的以及权重)
0.5 0.0   0.0   ! Z

0.5  0.0  0.0   ! Z
0.5 -0.5  0.0   ! K

0.5  -0.5 0.0   ! K
0.0 -0.5  0.0   ! L

0.0  -0.5 0.0   ! L
0.0  0.0  0.0   ! Γ
```

二维材料z方向仅取0的值




**Ref：10.1016/j.commatsci.2010.05.010**

**1、sumo**
**2、vaspkit**
**3、Online tool：**
**https://www.materialscloud.org/work/tools/seekpath**
**4、文献**

# 一、VASP的四个输入文件

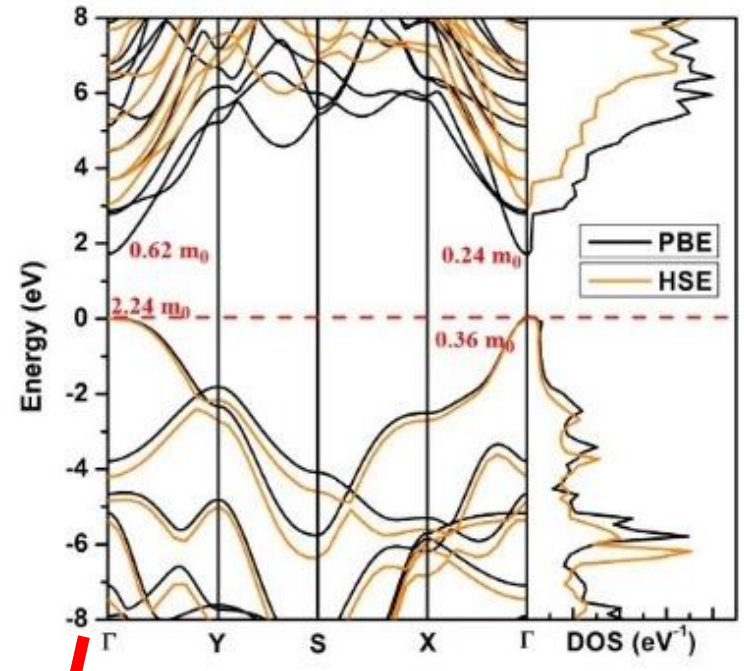
KPOINTS文件

3)手动定义各K点的坐标(一般仅在计算HSE能带结构时使用)：

```
Automatically generated mesh
      56
Reciprocal lattice
    0.00000000000000    0.00000000000000    0.00000000000000           1
    0.20000000000000    0.00000000000000    0.00000000000000           2
    0.40000000000000    0.00000000000000    0.00000000000000           2
    0.00000000000000    0.16666666666667    0.00000000000000           2
   -0.20000000000000    0.16666666666667    0.00000000000000           2
    0.00000000000000    0.50000000000000    0.00000000000000           1
    0.20000000000000    0.50000000000000    0.00000000000000           2
    0.40000000000000    0.50000000000000    0.00000000000000           2
0.   0.   0.0   0
0.05  0.   0.0   0
0.10  0.   0.0   0
0.15  0.   0.0   0
0.20  0.   0.0   0
0.25  0.   0.0   0
0.30  0.   0.0   0
0.35  0.   0.0   0
0.40  0.   0.0   0
0.45  0.   0.0   0
0.5 0.0 0.0   0
0.5 -0.05 0.0   0
0.5 -0.15 0.0   0
0.5 -0.20 0.0   0
0.5 -0.25 0.0   0
```

可以自己手写
可以vaspkit生成

来自IBZKPT文件




Ref：10.1039/c9tc02030f

用qvasp -bandd处理得到
dat文件，用origin画出

# 线性或HSE的KPOINTS产生器:vaspkit和sumo

```
+-------------------------------------------------------------+
|             VASPKIT Version: 0.70 (06 Nov. 2018)            |
|       A Pre- and Post-Processing Program for VASP Code      |
|       Official Website: http://vaspkit.sourceforge.net      |
|            Developed By Vei WANG (wangvei@me.com)           |
|            Contributor: Nan XU (tamas@zju.edu.cn)           |
+-------------------------------------------------------------+
====================== Structural Options =======================
1)  Customize INCAR File          2)  Elastic-Constant Calculator
3)  Poscar2other Toolkit          4)  Build Supercell
5)  Equation-of-State Fitting     6)  Structure Toolkit
7)  K-Mesh Generator              8)  Band-Path Generator

====================== Electronic Options =======================
11) Total Density-of-States       12) Projected Density-of-States
21) Band-Structure                22) Projected Band-Structure
23) 3D Band-Structure             25) Hybrid-DFT Band-Structure
26) Fermi-Surface Calculator

=========== Charge & Potential & Wavefunction Options ===========
31) Charge Density                32) Spin Density
33) Spin-Up & -Down Density       34) Charge-Density Difference
41) Planar-Average Charge-Density 42) Planar-Average Potential
51) Real-Space WaveFunction Plot

====================== Misc Utilities ===========================
71) Linear Optics                 72) Molecular-Dynamics Toolkit
73) VASP2BoltzTraP Interface      74) Energy-Related Toolkit
91) Semiconductor Calculator      92) 2D-Materials Toolkit

0)  Quit
------------>>
8
====================== Band-Path Options ========================
1) 1D Nano Structure
2) 2D Nano Structure
3) 3D bulk structure (Experimental)
```

```
[sunhr@mu01 ex01]$ sumo-kgen --seekpath
/public1/software/anaconda2/lib/python2.7/site-packages/pymatgen-2018.11.
Pymatgen will drop Py2k support from v2019.1.1. Pls consult the documenta
at https://www.pymatgen.org for more details.
  at https://www.pymatgen.org for more details.""")
Structure information:
        Space group number: 186
        International symbol: P6_3mc
        Lattice type: hexagonal

k-point path:
        \Gamma -> M -> K -> \Gamma -> A -> L -> H -> A | L -> M | H -> K

k-points:
        A: 0.0 0.0 0.5
        \Gamma: 0.0 0.0 0.0
        H: 0.333333333333 0.333333333333 0.5
        K: 0.333333333333 0.333333333333 0.0
        M: 0.5 0.0 0.0
        L: 0.5 0.0 0.5

k-point label indices:
        \Gamma: 1
        M: 71
        K: 112
        \Gamma: 193
        A: 231
        L: 301
        H: 342
        A: 423
        L: 424
        M: 462
        H: 463
        K: 501
```

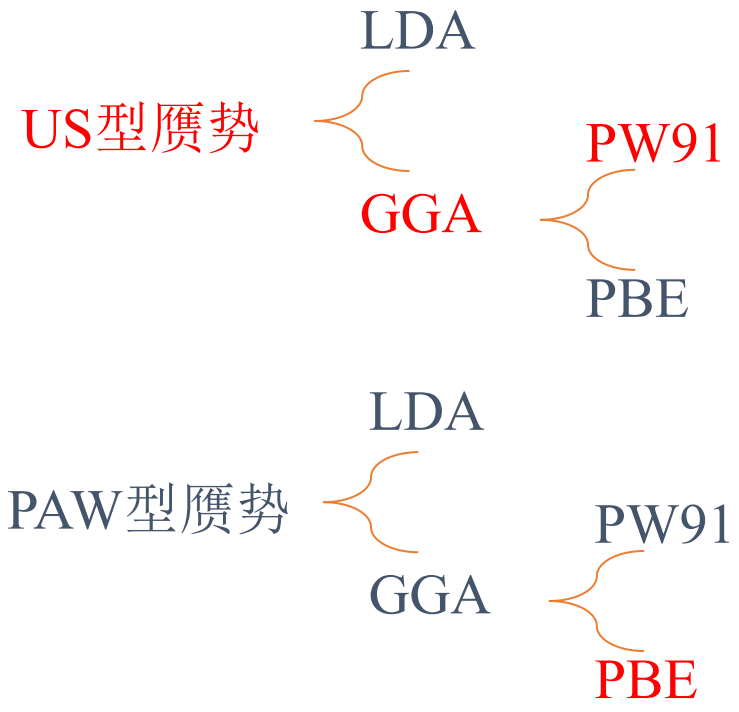
其它在线工具会在能带计算一章来讲

# 一、VASP的四个输入文件

POTCAR文件内容说明：

VASP程序本身有提供了赝势库，只需将体系各类原子的赝势合并在一起即可，但需注意到：

1）赝势类型：




US型赝势所需截至能较小，计算速度快，PAW赝势截至能通常较大，而且考虑的电子数多，计算慢，但精确度高。

**VASP已发布一种新泛函SCAN MetaGGA**

# 一、VASP的四个输入文件

* POTCAR中各原子赝势定义的顺序必需与POSCAR中相同：

```
surface of mgo(100) (2*2)Mg
   1.00000000000000
     5.9459999999999997    0.0000000000000000    0.0000000000000000
     0.0000000000000000    5.9459999999999997    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0000000000000000
  Al   N
  20  20
Selective dynamics
Direct
……
```

把Al的POTCAR和N的POTCAR合并成一个POTCAR文件即可，Al在前，N在后

* 对各原子的赝势参数，我们最关心的是截断能以及电子数;

* POTCAR的泛函类型必需与INCAR中GGA关键词定义的类型一致;

# 一、VASP的四个输入文件

POTCAR文件内容说明：


电子数目和组态

构造该赝势时，所采用的泛函类型，这里为PW91

对应于中等大小的截至能（构型优化时采用）

对应于低的截至能（动力学模拟时采用）

# POTCAR文件产生器

```
+=============================================================================================+
|                                        qvasp usage v2.21                                    |
|                                                    --Written by Wencai,Yi                   |
|                                                          2020.07.18                         |
+=================== POSCAR ================== + =============== POTCAR ======================+
| qvasp -fix  Fix atoms for POSCAR from *.vasp | qvasp -pw91 ELE_Name  POTCAR from PW91        |
| qvasp -t    Insert points for TS cal.(method1)| qvasp -pbe ELE_Name   POTCAR from PBE         |
| qvasp -t2   Insert points for TS cal.(method2)| qvasp -lda ELE_Name   POTCAR from LDA         |
| qvasp -sc   Create supercell for POSCAR      | qvasp -cp             Check the POTCAR        |
| qvasp -zc   Correct imaginary frequency      +================== KPOINTS ====================+
| qvasp -c2p  Transfer cif file to POSCAR      | qvasp -k number    Create KPOINTS(Auto mesh)   |
+=================== INCAR ================== + ================== Tools ======================+
| qvasp -relax   For Structure Optimization cal.| qvasp -gauss      Transfer OUTCAR to Gauss log |
| qvasp -ts      For Trasition State cal.       | qvasp -e          Read energy from OUTCAR      |
| qvasp -scf     For Self_Consistent cal.       | qvasp -p2c        Transfer format to *.cif     |
| qvasp -elf     For Eelectron Local Function   | qvasp -findcell   Find the pri-cell of CONTCAR |
| qvasp -wk      For Work Fuction cal.          | qvasp -wkd        Get Work Function from LOCPOT|
| qvasp -band    For Energy Band cal.           | qvasp -bandd      Deal Bands data from EIGENVAL|
| qvasp -dos     For Density Of States cal.     | qvasp -dosd       Deal DOS data from DOSCAR    |
| qvasp -bader   For Bader Charge cal.          | qvasp -ldos 1 2   Get LDOS data from DOS1 DOS2.|
| qvasp -hse     For HSE06 cal.                 | qvasp -mde        Read Energy data for AIMD    |
| qvasp -md      For Ab Init Molecular Dynamics | qvasp -mdm        Read Magnetic moment for AIMD|
| qvasp -elastic For Elastic Constants cal.     | qvasp -elasticd   Read elastic constants       |
| qvasp -partchg For PARTICAL Charge cal.       | qvasp -findsym    Find the symmetry            |
| qvasp -freq    For Frequency cal.             | qvasp -zpe        Get ZPE value                |
| qvasp -optics  For Optics Property cal.       | qvasp -opticsd    Get optics datas             |
| qvasp -phono   For Phonon Spectrum cal.       | qvasp -3dband     Get 3D band for 2D materials |
+================================== Customizable Tools =======================================+
| qvasp -nanotube POSCAR           Rolling nanosheet to POSCAR-nanotube                       |
| qvasp -out2arc                   Get trajectory file from OUTCAR to arc(opened by MS)       |
| qvasp -cleavesurface POSCAR      Cleave surface from POSCAR                                 |
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| qvasp -vaspkit                   Call VASPKIT program,ref:arXiv preprint arXiv:1908.08269   |
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+================================== Devoloper Info ===========================================+
| Cite with "The calculations were assisted by the qvasp code [1]"      QQ Group: 398274903      |
| [1] W. Yi, G. Tang, et al.qvasp: A Flexible Toolkit for VASP Users in Materials Simulations    |
+=============================================================================================+
```

**qvasp -pbe Al N将产生AlN的PAW_PBE的赝势POTCAR文件**

# 主要内容

一、VASP的四个输入文件

二、VASP的输出文件

三、与VASP相关搭配软件的使用

四、Linux下常用配套命令


VASP the GUIDE

# 二、VASP的输出文件

OUTCAR: 最主要的输出文件，包含了所有重要信息；

OSZICAR: 输出计算过程的能量迭代信息；

CONTCAR: 内容为最新一轮的构型(分数坐标，可用于续算)；

CHGCAR、CHG、PARCHG: 用于电荷密度图绘制；

WAVECAR: 波函数文件；

IBZKPT：具体的K点坐标信息

EIGENVAL: 记录各K点的能量本征值，用于绘制能带图；

XDATCAR: 构型迭代过程中各轮的构型信息(分数坐标，用于动力学模拟)；

DOSCAR: 态密度信息

# 主要内容

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VASP the GUIDE

# 三、与VASP相关搭配软件的使用

qvasp功能

```
+=============================================================================================+
|                                      qvasp usage v2.21                                      |
|                                                    --Written by Wencai,Yi                   |
|                                                         2020.07.18                          |
+=================== POSCAR =================== + =============== POTCAR =====================+
| qvasp -fix  Fix atoms for POSCAR from *.vasp  | qvasp -pw91 ELE_Name  POTCAR from PW91        |
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| [1] W. Yi, G. Tang, et al.qvasp: A Flexible Toolkit for VASP Users in Materials Simulations |
+=============================================================================================+
```

# 三、与VASP相关搭配软件的使用

## vaspkit

```
[sunhr@mu01 software]$ vaspkit

 +-------------------------------------------------------------+
 |             VASPKIT Version: 0.70 (06 Nov. 2018)            |
 |       A Pre- and Post-Processing Program for VASP Code      |
 |       Official Website: http://vaspkit.sourceforge.net      |
 |            Developed By Vei WANG (wangvei@me.com)           |
 |            Contributor: Nan XU (tamas@zju.edu.cn)           |
 +-------------------------------------------------------------+
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 5)  Equation-of-State Fitting     6)  Structure Toolkit
 7)  K-Mesh Generator              8)  Band-Path Generator

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 =========== Charge & Potential & Wavefunction Options ==========
 31) Charge Density                32) Spin Density
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 41) Planar-Average Charge-Density 42) Planar-Average Potential
 51) Real-Space WaveFunction Plot

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 71) Linear Optics                 72) Molecular-Dynamics Toolkit
 73) VASP2BoltzTraP Interface      74) Energy-Related Toolkit
 91) Semiconductor Calculator      92) 2D-Materials Toolkit

 0)  Quit
 ------------>>
```

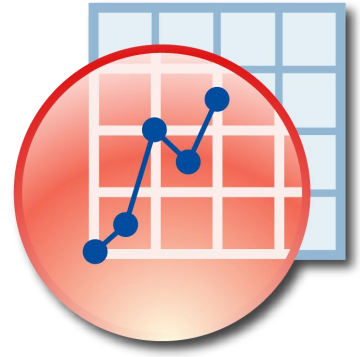


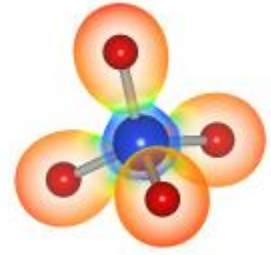

VESTA

Visualization for Electronic and STructural Analysis


Virtual NanoLab 2015.1


ChemDraw

# 主要内容

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VASP the GUIDE

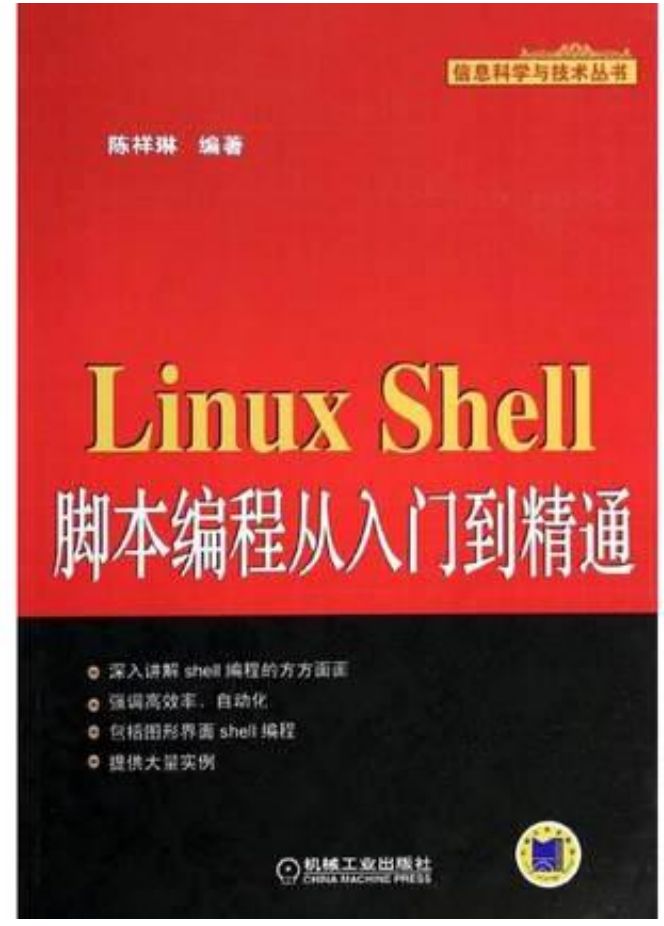
# 四、Linux下常用配套命令

1、vi编辑器的使用

2、正则表达(awk/grep/sed等)

3、脚本编写(for-do-done)与批处理

参考右侧书内容




**这在日常工作中用到的频率很高，建议掌握！**

# 第三讲 结构建模基础

易文才

# 前情提要

1、计算模型坏，**后面全歇菜**

2、理解周期性概念（面心，顶角：金刚石为例）

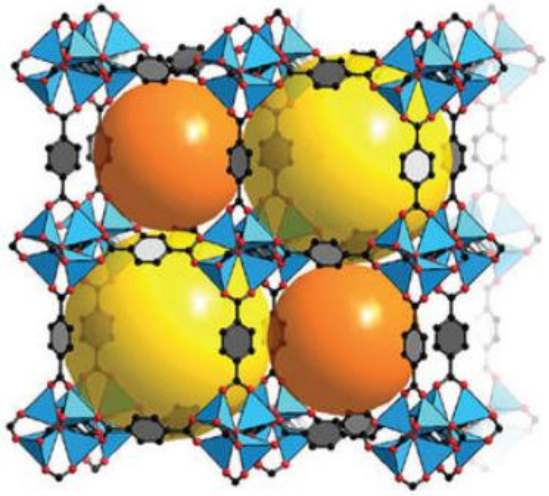
3、坐标比视图更重要，分清楚

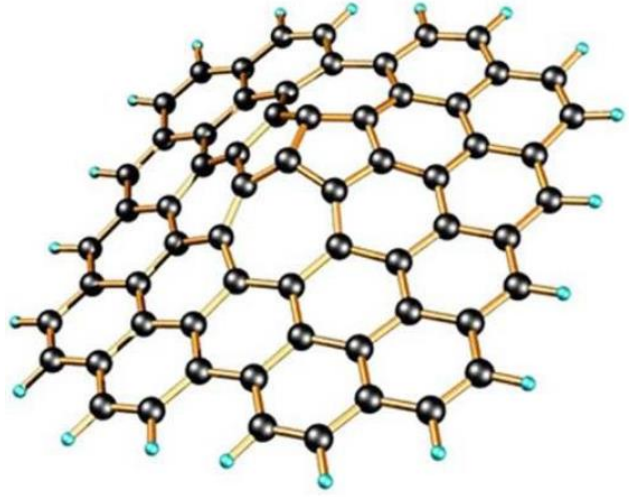
4、建模步骤不重要，手段不重要，最终能够得到正确的原子晶格和坐标信息即可

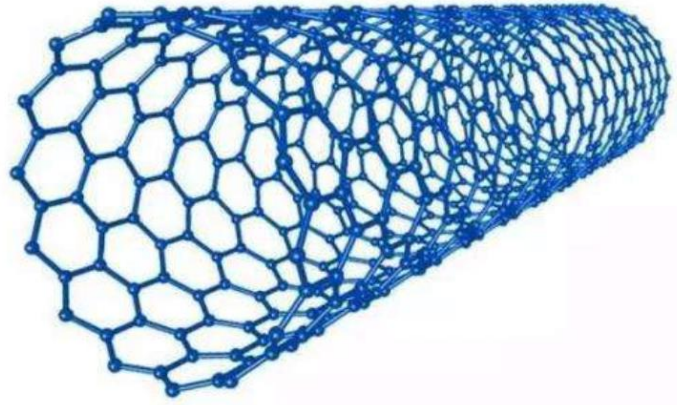
5、三思而后问，先查而后问

# 计算模型有多重要？

- 几乎所有的材料计算模拟都是从建模开始的







# 主要内容

一、建模软件和晶胞获取

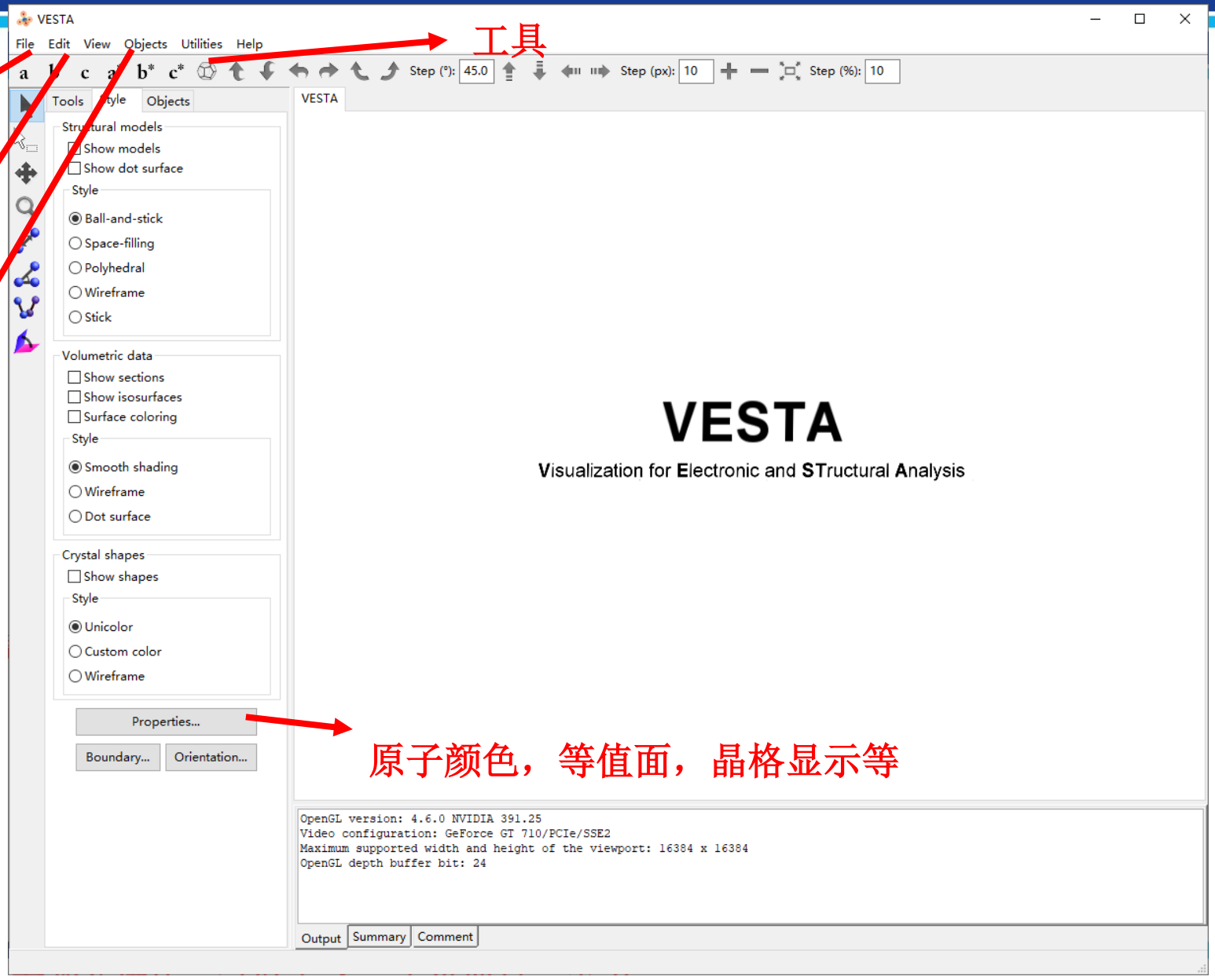
二、构建二维材料

三、掺杂、缺陷、空位

四、切表面、单原子催化剂、共吸附模型

五、异质结和纳米管模型

# VESTA界面初识别




工具

新建
存文件
导图

编辑

边界

原子颜色，等值面，晶格显示等

存储图片质量极高
电荷密度极好看

# 一、晶胞(Unit Cell)获取的方法

**软件自带、晶体数据库**和**文献（支持信息）**

常见的晶体数据库：**下载cif文件，以上所涉软件都能打开**

1、晶体开放数据库：http://www.crystallography.net/cod/search.html

2、Materials Project：https://www.materialsproject.org/

3、美国矿物晶体数据库：http://rruff.geo.arizona.edu/AMS/amcsd.php

4、ChEBI：https://www.ebi.ac.uk/chebi/init.do

5、AFLOW：http://www.aflow.org/

6、Springer Materials: http://materials.springer.com/

相信在材料基因计划的驱使下，未来中国也会有很多数据库

# COD晶体库搜索示例

## Search

(For more information on search see the hints and tips)

| Search by COD ID: | Search |
|---|---|

| OpenBabel FastSearch: | Enter SMILES: Search |
|---|---|

ubstructure search by SMILES is currently available in a subset of COD containing 1784

| | |
|---|---|
| text (1 or 2 words) | |
| journal | |
| year | |
| volume | |
| issue | |
| DOI | |
| Z (min, max) | |
| Z' (min, max) | |
| chemical formula (in Hill notation) | |
| 1 to 8 elements | Sr Ti O |
| NOT these elements | N H S C |
| volume min and max | |
| number of distinct elements min and max | |
| filters | has $F_{obs}$<br>include duplicate entries<br>include entries with errors<br>include theoretical structures |
| Reset | Send |

## $SrTiO_3$晶体结构搜索

| | | | | | | |
|---|---|---|---|---|---|---|
| | HKL Paper | | | 10.5585<br>90; 90; 90 | | Dopant positions in strontium/chromium- and barium-doped K radiation<br>*Acta Crystallographica Section B*, **2000**, *56*, 90 |
| 2102732 | CIF Paper | Cr Li O11 Sr Ti4 | P n m a | 13.818; 5.755; 9.901<br>90; 90; 90 | 787.35 | Imaz, Inhar; Pechev, Stanislav; Gravereau, Pierre; Chaminade, Jea Bouree, Francoise<br>Structural filiations in the new complex titanates SrLiMT<br>*Acta Crystallographica Section B*, **2007**, *63*, 26-36 |
| 2102733 | CIF Paper | Cr Li O11 Sr Ti4 | P n m a | 13.798; 5.763; 9.89<br>90; 90; 90 | 786.4 | Imaz, Inhar; Pechev, Stanislav; Gravereau, Pierre; Chaminade, Jea Bouree, Francoise<br>Structural filiations in the new complex titanates SrLiMT<br>*Acta Crystallographica Section B*, **2007**, *63*, 26-36 |
| 2102734 | CIF Paper | Fe Li O11 Sr Ti4 | P b c n | 13.875; 11.492; 19.887<br>90; 90; 90 | 3171 | Imaz, Inhar; Pechev, Stanislav; Gravereau, Pierre; Chaminade, Jea Bouree, Francoise<br>Structural filiations in the new complex titanates SrLiMT<br>*Acta Crystallographica Section B*, **2007**, *63*, 26-36 |
| 2237244 | CIF Paper | O8 Si2 Sr2 Ti | P 4 b m | 8.32; 8.32; 5.0239<br>90; 90; 90 | 347.77 | Bell, Anthony M. T.; Henderson, C. Michael B.<br>Sr-fresnoite determined from synchrotron X-ray powder diffrac<br>*Acta Crystallographica Section E*, **2013**, *69*, i1 |
| 2310687 | CIF | O3 Sr Ti | I 4/m c m | 5.511; 5.511; 7.796<br>90; 90; 90 | 236.773 | Tsuda, K.; Tanaka, M.<br>Refinement of crystal structure parameters using convergent-be temperature phase of SrTiO~3~<br>*Acta Crystallographica Section A*, **1995**, *51*, 7-19 |
| 4000094 | CIF | Na0.8 O7.6 Si2.4 Sr0.8 Ti | C m m m | 23.19; 7.2259; 6.9699<br>90; 90; 90 | 1167.9 | *Chemistry of Materials*, **2001** |
| 4000485 | CIF | Cu3 O12 Sr Ti4 | I m -3 | 7.42757; 7.42757; 7.42757<br>90; 90; 90 | 409.769 | Li, J; Subramanianb, M A; Rosenfeldb, H D; Jones, C Y; Toby, B H<br>*Chemistry of Materials*, **2004** |
| 4000873 | CIF | Ce0.4 O3 Sr0.4 Ti | C 1 2/c 1 | 9.5228; 5.4869; 5.4818<br>90; 125.222; 90 | 233.99 | Ubic, Rick; Subodh, Ganesanpotti; Gout, Delphine; Sebastian, Ma<br>Correction to Crystal Structure of Sr0.4Ce0.4TiO3Ceramics<br>*Chemistry of Materials*, **2010**, *22*, 2174 |
| 4001057 | CIF | Ce0.4 O3 Sr0.4 Ti | C 1 2/c 1 | 9.5228; 5.4869; 5.4818<br>90; 125.222; 90 | 233.99 | Ubic, Rick; Subodh, Ganesanpotti; Gout, Delphine; Sebastian, Ma<br>Crystal Structure of Sr0.4Ce0.4TiO3Ceramics<br>*Chemistry of Materials*, **2009**, *21*, 4706 |
| 4001153 | CIF | Ce0.445 O3 Sr0.352 Ti | R -3 c :H | 5.486; 5.486; 13.4539<br>90; 90; 120 | 350.663 | Ubic, Rick; Subodh, Ganesanpotti; Sebastian, Mailadil T.; Gout, D<br>Structure of Compounds in the Sr1-3x/2CexTiO3Homologous S<br>*Chemistry of Materials*, **2008**, *20*, 3127 |
| 4001154 | CIF | Ce0.269 O3 Sr0.601 Ti | R -3 c :H | 5.5005; 5.5005; 13.4797<br>90; 90; 120 | 353.196 | Ubic, Rick; Subodh, Ganesanpotti; Sebastian, Mailadil T.; Gout, D<br>Structure of Compounds in the Sr1-3x/2CexTiO3Homologous S<br>*Chemistry of Materials*, **2008**, *20*, 3127 |
| 4001155 | CIF | Ce0.167 O3 Sr0.744 Ti | R -3 c :H | 5.5062; 5.5062; 13.4989<br>90; 90; 120 | 354.432 | Ubic, Rick; Subodh, Ganesanpotti; Sebastian, Mailadil T.; Gout, D<br>Structure of Compounds in the Sr1-3x/2CexTiO3Homologous S<br>*Chemistry of Materials*, **2008**, *20*, 3127 |
| 4001156 | CIF | Ce0.133 O3 Sr0.795 Ti | R -3 c :H | 5.5091; 5.5091; 13.5071<br>90; 90; 120 | 355.021 | Ubic, Rick; Subodh, Ganesanpotti; Sebastian, Mailadil T.; Gout, D<br>Structure of Compounds in the Sr1-3x/2CexTiO3Homologous S<br>*Chemistry of Materials*, **2008**, *20*, 3127 |
| 4002469 | CIF | Cu0.5 La0.5 O3.78 Sr1.5 Ti0.5 | P 4 2 2 | 5.447; 5.447; 12.7693 | 378.863 | Byeon, S.H.; Chung, H.<br>Investigation of the Ruddlesden-Popper oxygen pressure induced |

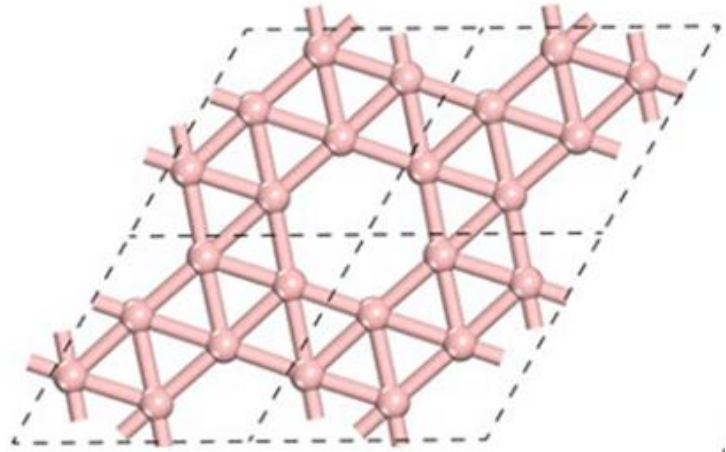
# 二、晶胞(Unit Cell)获取的方法

文献：

查询文献的Supporting Information

获取结构参数（晶格常数，原子坐标 (空间群)）

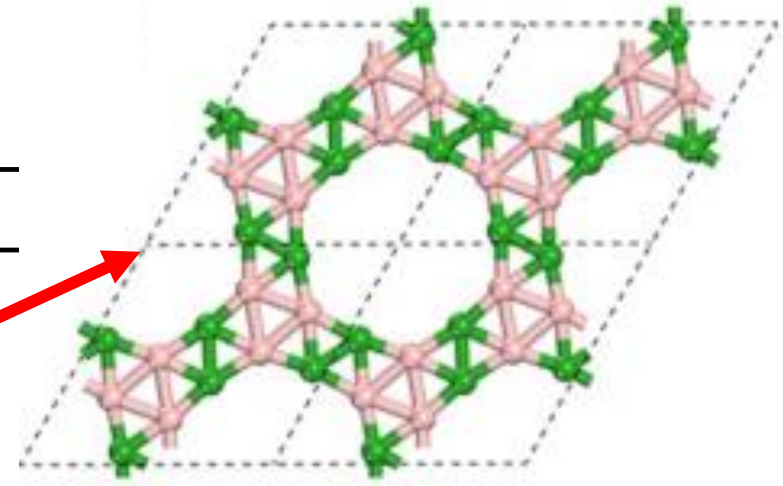
使用软件建模



Example：

DOI:10.1021/acs.jpclett.7b00891

| Allotrope | a (Å) | Space group | Atomic positions |
|---|---|---|---|
| χ-$h_0$ | 4.47 | *P6/m* | B1(0.718 0.146 0.500) |
| χ-$h_1$ | 7.31 | *P6/m* | B1(0.694 0.207 0.500) B2(0.058 0.625 0.500) |
| χ-$h_2$ | 10.05 | *P-3* | B1(0.681 0.239 0.496) B2(0.133 0.642 0.516) B3(0.544 0.595 0.490) |



# 实例演示：VESTA对χ-$h_1$单层的建模

# 主要内容

一、建模软件和晶胞获取

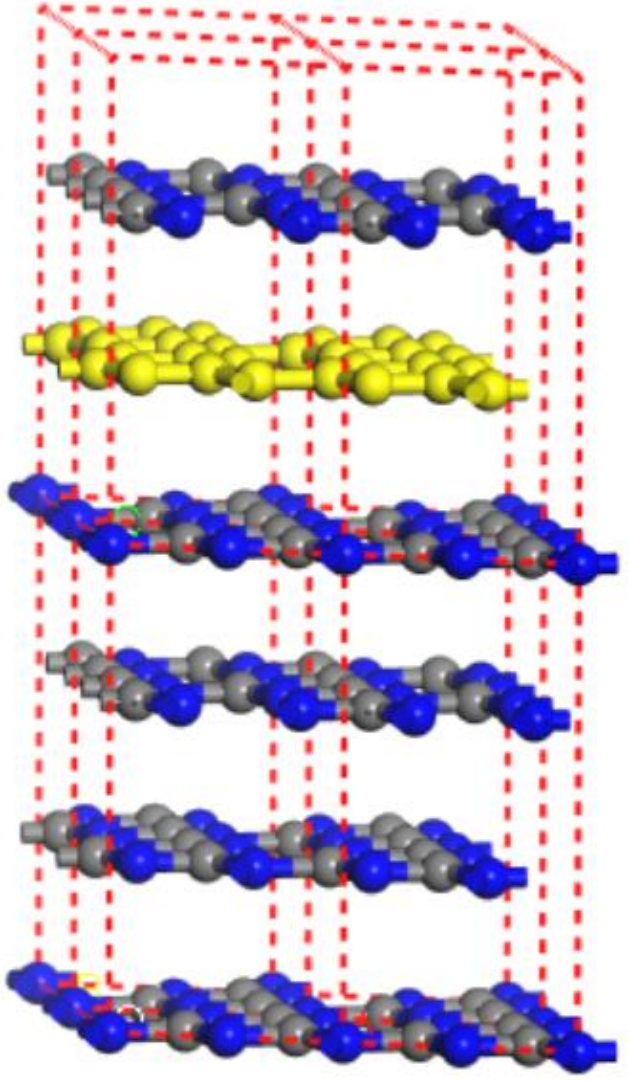
二、构建二维材料

三、掺杂、缺陷、空位

四、切表面、单原子催化剂、共吸附模型

五、异质结和纳米管模型

# 二、从层状材料剥离二维材料



g-$C_3N_4$

剥离步骤：

1、找到该层状材料晶体结构

2、选中多余的层

3、删掉

4、加真空层

# 主要内容

一、建模软件和晶胞获取

二、构建二维材料

三、掺杂、缺陷、空位

四、切表面、单原子催化剂、共吸附模型

五、异质结和纳米管模型

# 实例演示：VESTA对缺陷、空位、掺杂的构造

# 主要内容

一、建模软件和晶胞获取

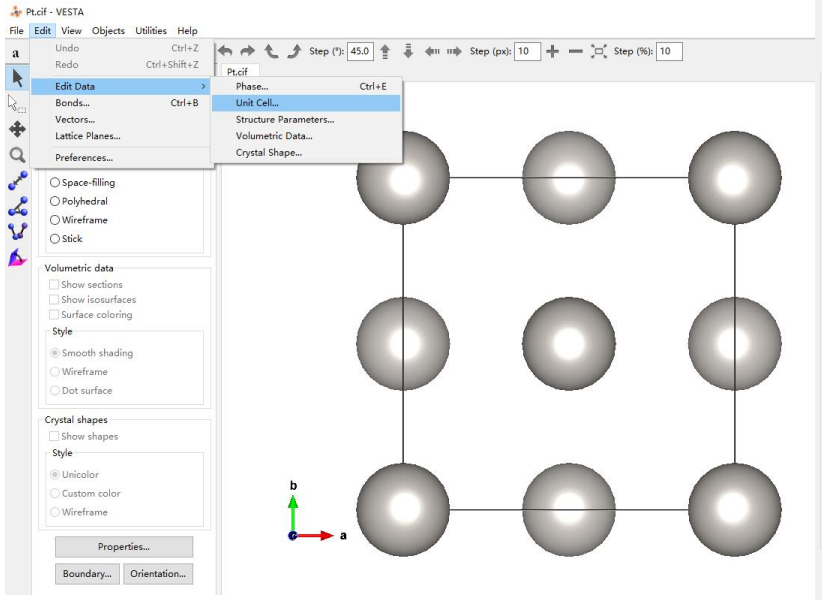
二、构建二维材料

三、掺杂、缺陷、空位

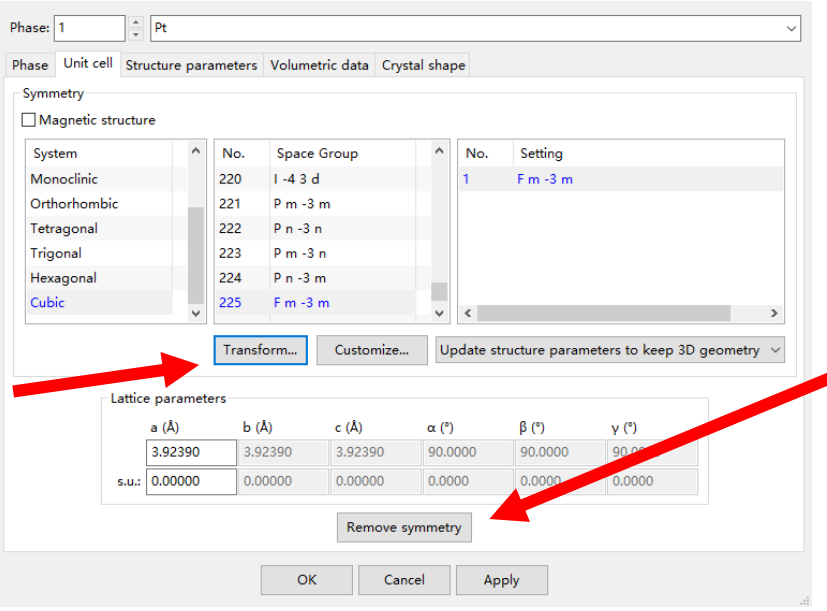
**四、切表面、单原子催化剂、共吸附模型**

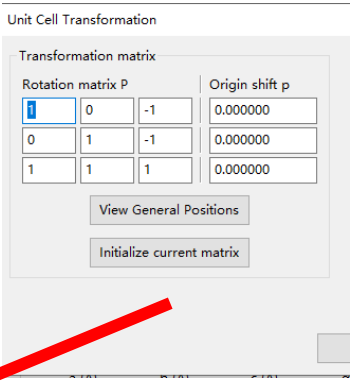
五、异质结和纳米管模型

# 四、切表面

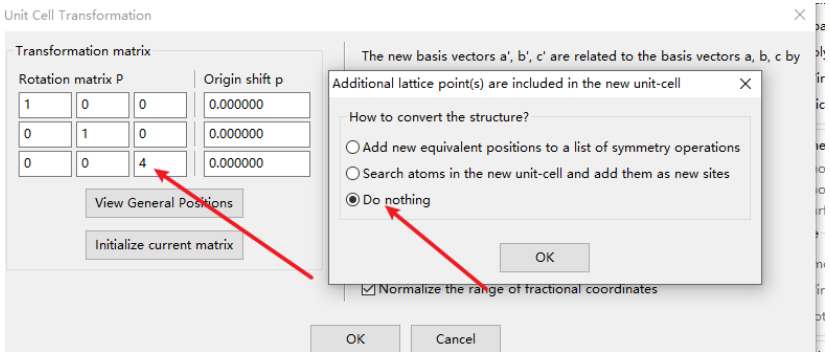



使用惯胞切面

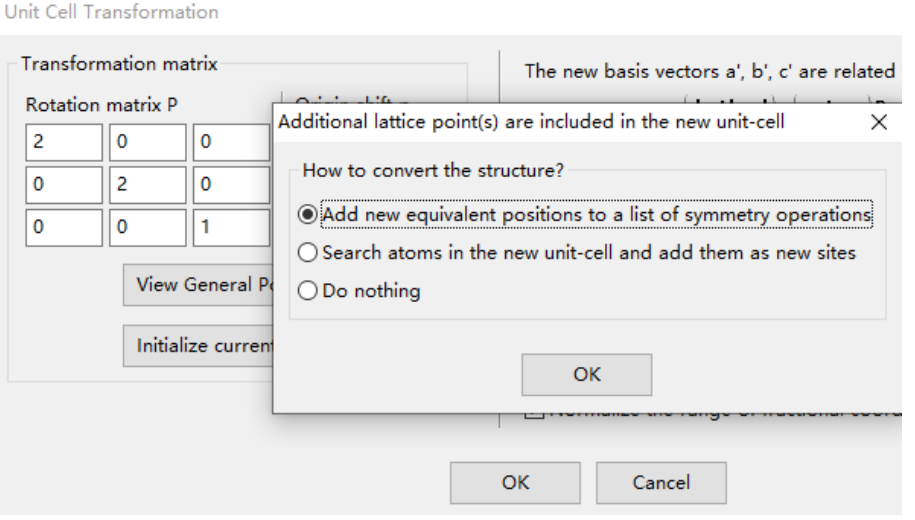



切111面,计算晶格矢量

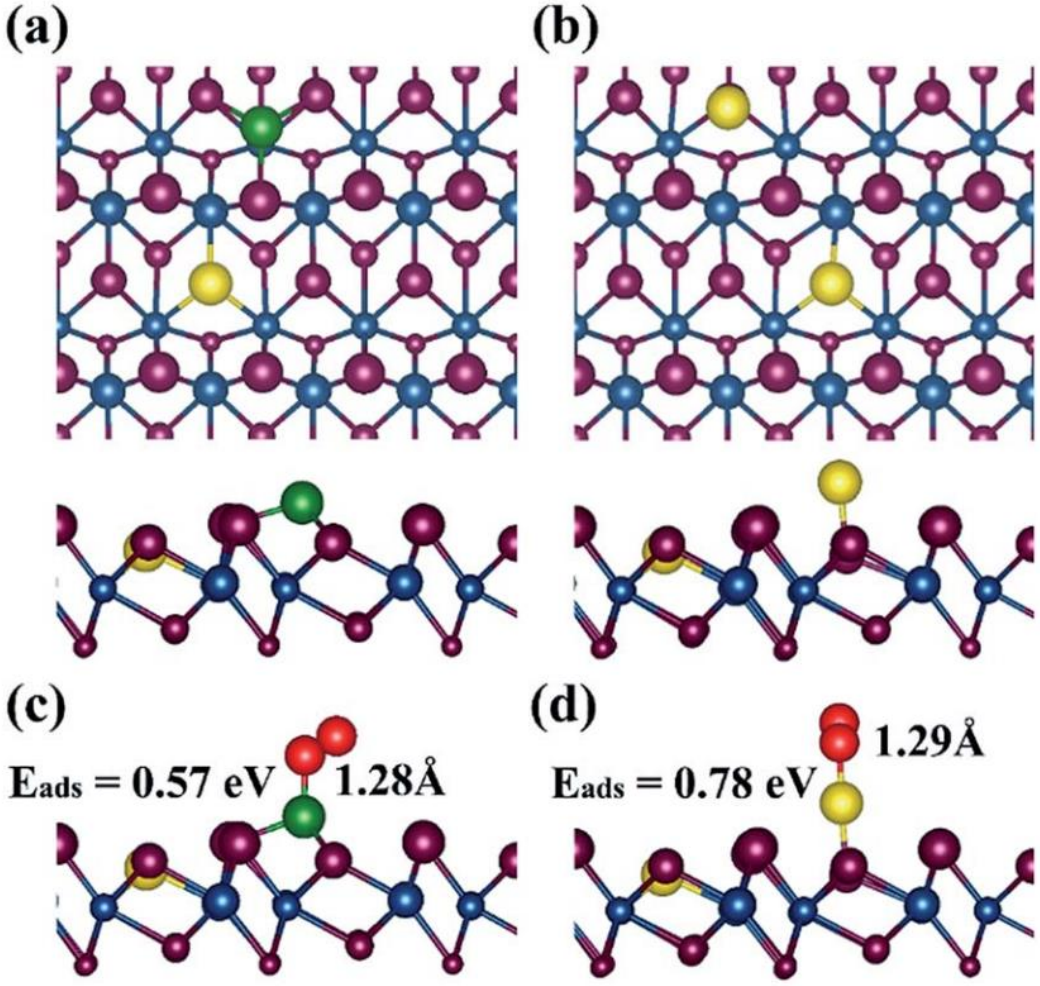



加真空层厚度




扩2x2超胞

# 四、单原子催化、共吸附模型




*J. Mater. Chem. A*, 2019,7, 9297-9304

单原子催化表面模型：
1、切表面
2、在表面添加单原子，优化

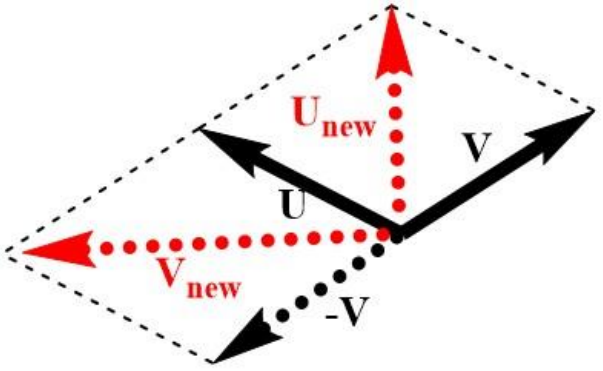
共吸附模型：
1、切表面，优化。
2、创建小分子模型，优化。
3、复制小分子原子结构，粘贴到表面上，调整到恰当位置，优化。

# 四、根号乘根号表面的由来

- 切面多大尺寸合适
- 纯金属切面，以Pt(111)为例
- 如何定义根号乘根号的面

切面可以用Materials studio或者VNL

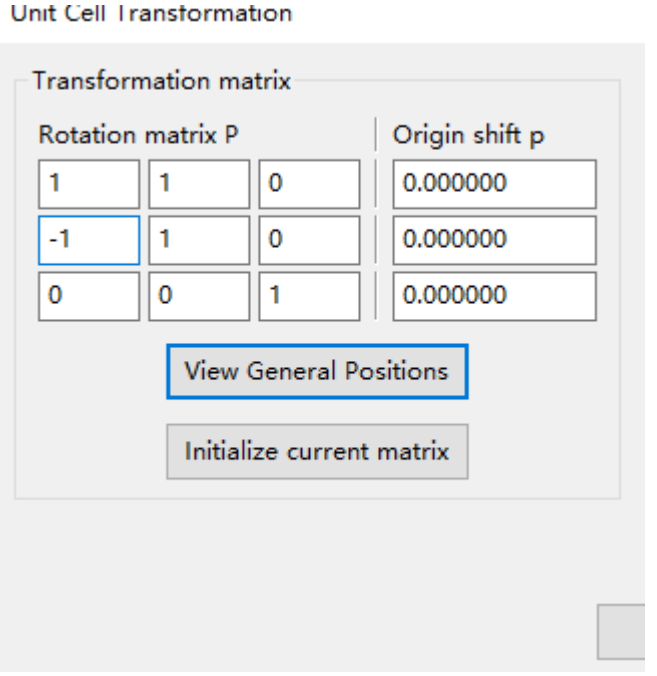
注意使用（U V）值来构建根号乘根号的面

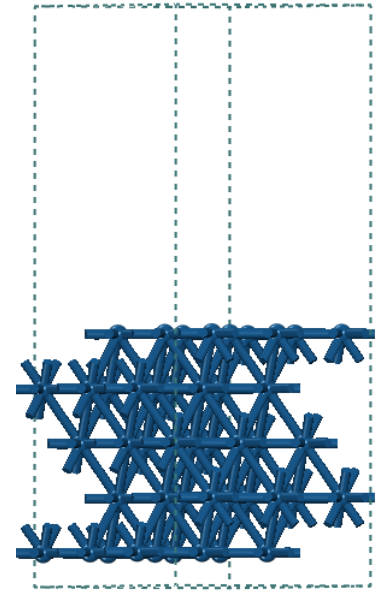



U和V：$a$

$U_{new}$: $a$　$V_{new}$: $\sqrt{3}a$

结果：Pt111 2x2$\sqrt{3}$



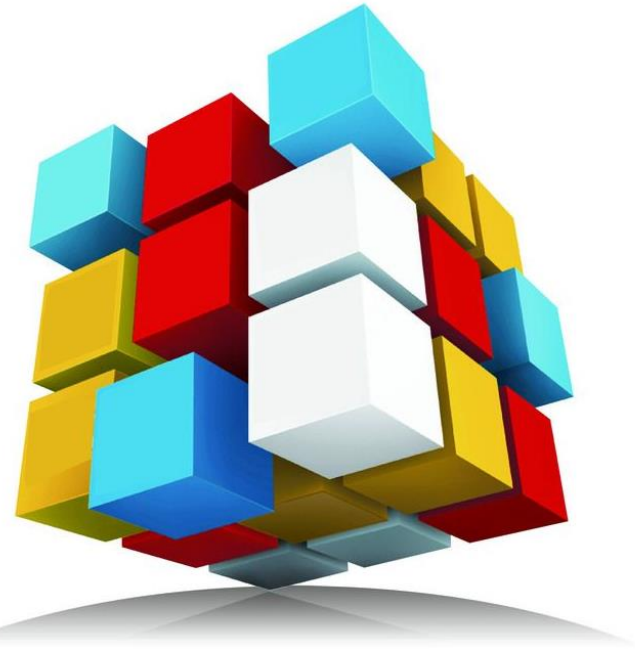



# 主要内容

一、建模软件和晶胞获取

二、构建二维材料

三、掺杂、缺陷、空位

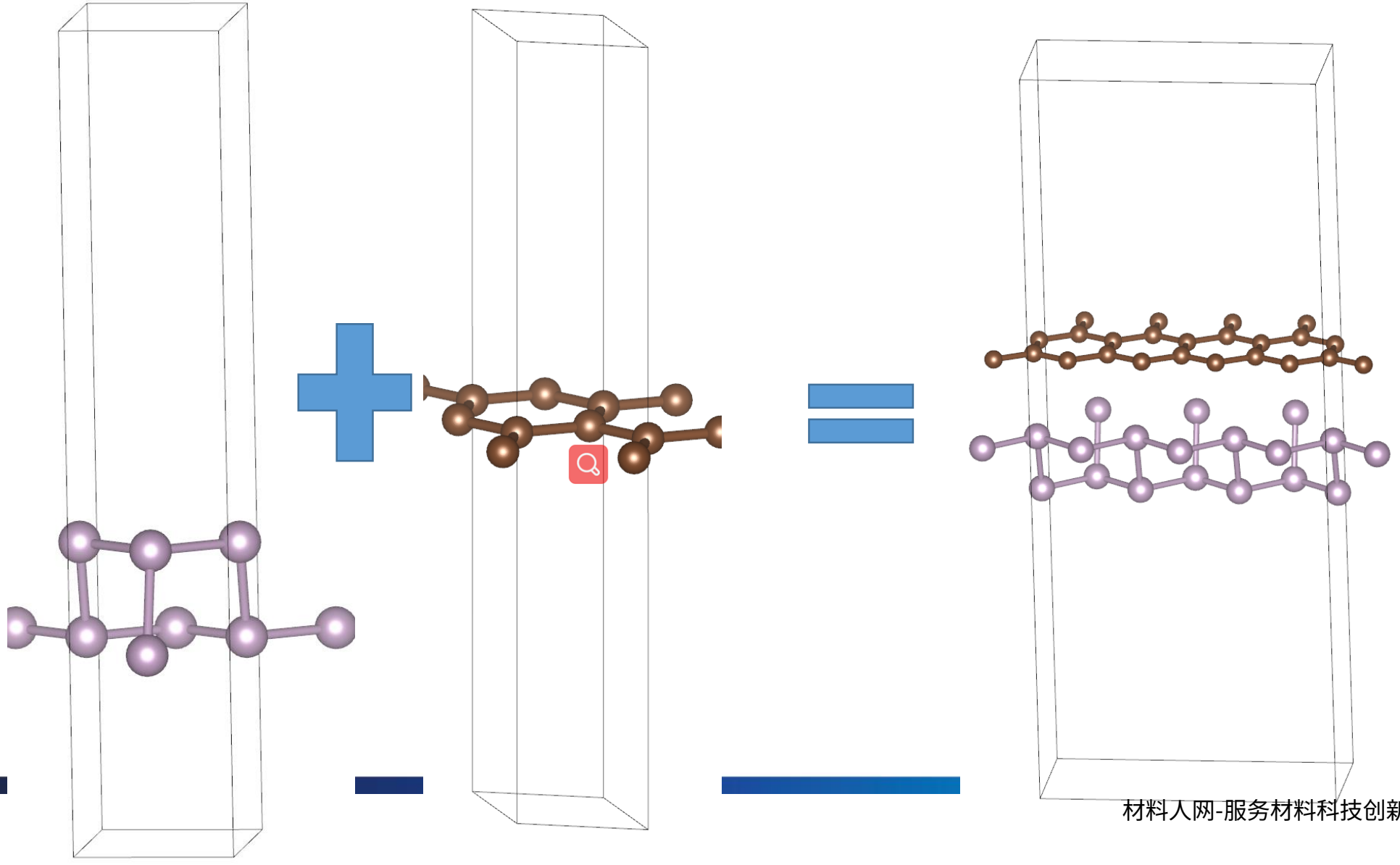


四、切表面、单原子催化剂、共吸附模型

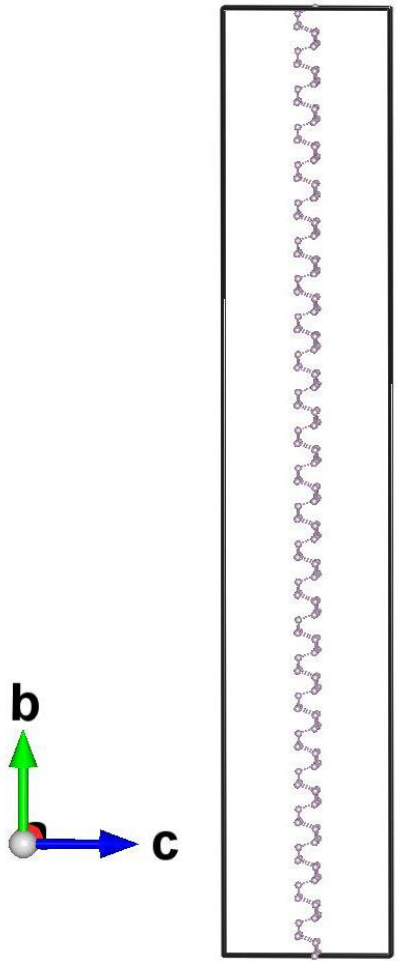
**五、异质结和纳米管模型**

# 五、异质结和纳米管模型

补充免费工具：来自vaspkit异质结建模杯获奖作品脚本



# 五、异质结和纳米管模型

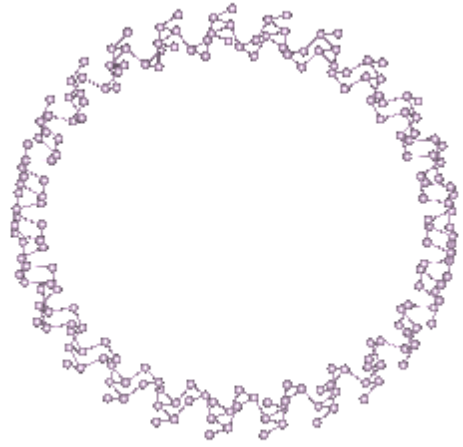



1、先建立方形的模型，以便进行弯曲成圆。

2、导出成POSCAR坐标（笛卡尔坐标形式）

3、转换坐标，使**b轴为长轴，c轴为真空方向，a轴为弯曲轴**

4、使用qvasp –nanotube POSCAR对结构进行弯曲，生成POSCAR-nanotube



# 思考、回顾和练习

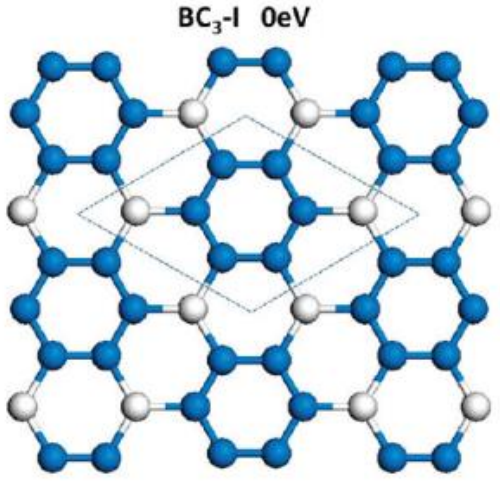
思考：

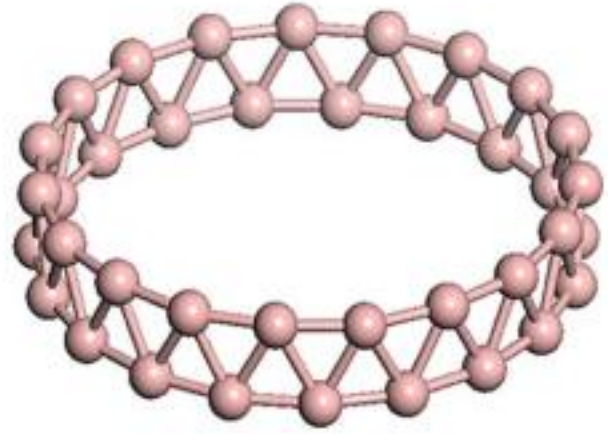
1、固体表面的切面，表面终端是唯一的吗？以$Co_2O_3$为例

练习：

1、搜索$SrTiO_3$的晶体结构

2、搭建下面的结构



# 第四讲 VASP参数收敛性测试

易文才

# 一、前言：测试目的与准备

测试前的目的

## 计算精度 PK 计算时间

# 一、测试目的与准备:测试必要性

## 1、ENCUT

平面波的切断动能。在任何性质的计算之前，进行ENCUT收敛情况的计算，由此来确定一个合适的切断动能值，然后手动地设置。

*Can you rely on the default cutoff ?*

it depends

- ENCUT is a very reasonable compromise between accuracy and speed
- you can rely on ENCUT, as long as the
  - cell-shape and the volume remain unchanged
  - frozen phonon calculations
  - surface and slab calculations
  - adsorption of molecules on surfaces
- otherwise you might need to be rather careful

# 一、测试目的与准备:测试必要性

**Mind:** Before you perform relaxations in which the volume or the cell shape is allowed to change you must read and understand the section on energy vs. volume, volume relaxations, and Pulay stress. In general volume changes should be done only with an increased energy cutoff, *i.e.*, ENCUT=1.3×max(ENMAX) or PREC=High.

```
 PAW Si 02Apr1999
  4.00000000000000
parameters from PSCTR are:
  VRHFIN =Si: s2p2
  LEXCH  = CA
  EATOM  =   103.4324 eV,    7.6021 Ry

  TITEL  = PAW Si 02Apr1999
  LULTRA =        F    use ultrasoft PP ?
  IUNSCR =        1    unscreen: 0-lin 1-nonlin 2-no
  RPACOR =    1.500    partial core radius
  POMASS =   28.085; ZVAL   =    4.000    mass and valenz
  RCORE  =    1.900    outmost cutoff radius
  RWIGS  =    2.48 ; RWIGS  =    1.312    wigner-seitz radius (au A)
  ENMAX  =  245.704; ENMIN  =  184.278 eV
```

http://cms.mpi.univie.ac.at/vasp/vasp/Volume_vs_energy_volume_relaxations_Pulay_Stress.html

http://www.bigbrosci.cn/newsitem/278019758

# 一、测试目的与准备:测试必要性

## 2、KPOINTS

计算完后得到k点数目与能量的对应值，总能变化在0.001eV/atom左右就非常足够了，然后由此来选择合适的k点数目。

Number of k-points, and method for smearing

*Read and understand section 7.4 before reading this section.*

The number of k-points necessary for a calculation depends critically on the necessary precision and on the fact whether the system is metallic. Metallic systems require an order of magnitude more k-points than semiconducting and insulating systems. The number of k-points also depends on the smearing method in use; not all methods converge with similar speed. In addition the error is not transferable at all i.e. a $9 \times 9 \times 9$ leads to a completely different error for fcc, bcc and sc. Therefore absolute convergence with respect to the number of k-points is necessary. The only exception are commensurable super cells. If it is possible to use the same super cell for two calculations it is definitely a good idea to use the same k-point set for both calculations.

k-point mesh and smearing are closely connected. We repeat here the guidelines for ISMEAR already given in section 6.38:

- For semiconductors or insulators always use tetrahedron method (ISMEAR=-5), if the cell is too large to use tetrahedron method use ISMEAR=0.
- For relaxations *in metals* always use ISMEAR=1 and an appropriated SIGMA value (so that the entropy term is less than 1 meV per atom). *Mind:* Avoid to use ISMEAR＞0 for semiconductors and insulators, it might result in problems.
- For the DOS and very accurate *total energy* calculations (no relaxation in metals) use the tetrahedron method (ISMEAR=-5).

The number of k-points necessary for a calculation depends critically on the necessary precision and on the fact whether the system is metallic. Metallic systems require an order of magnitude more k-points than semiconducting and insulating systems. The number of k-points also depends on the smearing method in use; not all methods converge with similar speed. In addition the error is not transferable at all i.e. a 9*9*9 leads to a completely different error for fcc, bcc and sc. Therefore absolute convergence with respect to the number of k-points is necessary. The only exception are commensurable super cells. If it is possible to use the same super cell for two calculations it is definitely a good idea to use the same k-point set for both calculations.

# 一、测试目的与准备:测试必要性

**Hint**

A rule of thumb for choosing the initial **k**-point sampling is, that the product, *ka*, between the number of **k**-points, *k*, in any direction, and the length of the basis vector in this direction, *a*, should be:

- *ka* ~ 30 Å, for *d* band metals
- *ka* ~ 25 Å, for simple metals
- *ka* ~ 20 Å, for semiconductors
- *ka* ~ 15 Å, for insulators

Remember that convergence in this parameter should always be checked.

https://www.bigbrosci.com/categories/LVASPTHW/

# 一、测试目的与准备:测试必要性

ENCUT=300 eV

```
Stiffness Tensor C_ij (in GPa):
   159.587     63.382     63.382      0.000      0.000      0.000
    63.382    159.587     63.382      0.000      0.000      0.000
    63.382     63.382    159.587      0.000      0.000      0.000
     0.000      0.000      0.000     75.250      0.000      0.000
     0.000      0.000      0.000      0.000     75.250      0.000
     0.000      0.000      0.000      0.000      0.000     75.250
```

ENCUT=600 eV

```
Stiffness Tensor C_ij (in GPa):
   158.776     63.501     63.501      0.000      0.000      0.000
    63.501    158.776     63.501      0.000      0.000      0.000
    63.501     63.501    158.776      0.000      0.000      0.000
     0.000      0.000      0.000     74.888      0.000      0.000
     0.000      0.000      0.000      0.000     74.888      0.000
     0.000      0.000      0.000      0.000      0.000     74.888
```

Si的弹性模量计算

# 一、前言：测试目的与准备

测试前的准备

- 查阅是否有类似计算体系的文章？
  若有，可参考文献上的参数值即可

- 准备测试的文件
  INCAR, KPOINTS, POSCAR, POTCAR,提交任务的脚本

区分概念：原胞、单胞、惯胞、超胞
如果通过phonopy得到标准基矢

phonopy –symmetry --tolerance **0.1**

# 脚本准备

需要掌握的编程知识：

1、for循环的使用

2、如何利用cat命令生成一个文件

3、如何提取OUTCAR中的能量(grep/tail/awk组合使用)

have the same number of distinct points to examine in the IBZ. This occurs because in the Monkhorst–Pack approach using an odd value of $M$ includes some $k$ points that lie on the boundaries of the IBZ (e.g., at the Γ point) while even values of $M$ only give $k$ points inside the IBZ. An implication of

```
# for i in `seq 3 9`
for i in 3 4 5 6 7 8 9
do
cat > KPOINTS << !
auto
0
Gamma
$i $i $i
0.0 0.0 0.0
!

echo "K=$i " ; /home/tg/intel/impi/2018.0.128/intel64/bin/mpirun  -np 8  $EXEC
E=$(grep "TOTEN" OUTCAR | tail -1 | awk '{printf  "%12.6f \n", $5 }')
K=$(grep "irred" OUTCAR | tail -1 | awk '{printf "%4i\n", $2 }')
echo $i  $E  >> kpoints_test.dat
done
```

cat > filename << EOF

XXXXXXX

EOF

%12.6f 表示输出字段宽度为12的浮点数，其中小数位为6。

写到提交任务的脚本如PBS等

http://blog.sina.com.cn/s/blog_587b601c0102vhot.html

https://zhidao.baidu.com/question/1946163069668139428.html

http://wiki.tangzeyuan.com/software/vasp-scripts.html#energy-cutoff-test

# 脚本准备

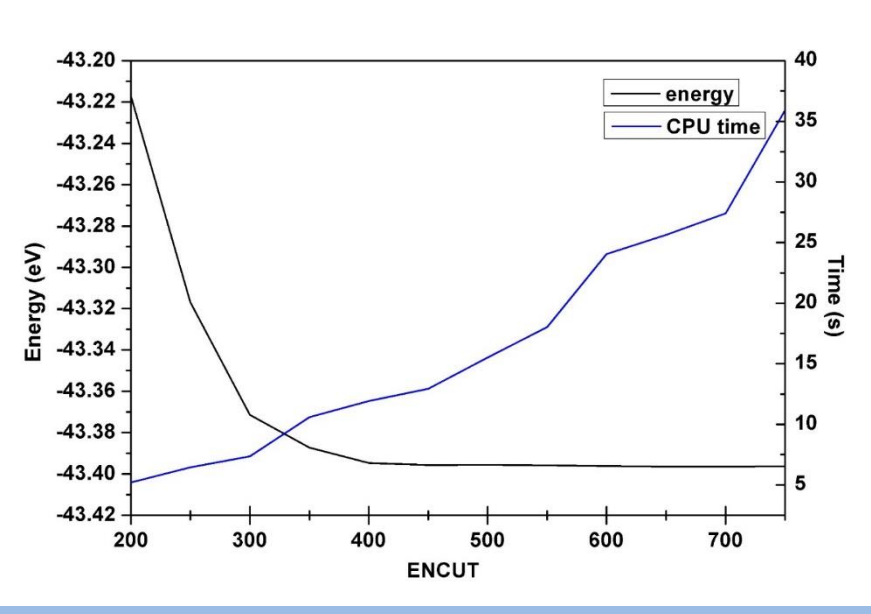
```
# for i in `seq 300 50 700`
for i in 300 350 400 450 500 550 600 650 700 750 800
do
cat > INCAR <<!
SYSTEM=Si
PREC = Accurate
KSPACING = 0.2

IBRION = 1
ISIF   = 2

ISMEAR = -5
NSW    = 0

EDIFF  = 1E-5
ENCUT = $i

LWAVE = .FALSE.
LCHARG = .FALSE.
!
E=$(grep "TOTEN" OUTCAR | tail -1 | awk '{printf  "%12.6f \n", $5 }')
echo "ENCUT=$i eV " ; /home/tg/intel/impi/2018.0.128/intel64/bin/mpirun  -np 8  $EXEC
E=$(grep "TOTEN" OUTCAR | tail -1 | awk '{printf  "%12.6f \n", $5 }')
echo $i  $E  >> encut_test.dat
done
```

# 三、截断能的测试和SIGMA测试

## ENCUT测试

- 脚本

```
for i in 260 280 300 320 340 360 380 400 420 460 500
do
cat > INCAR <<!
SYSTEM = Rutile
ENCUT = $i
…….
!
echo "ENCUT= $i eV";
rm -f WAVECAR CHGCAR
run vasp
E=`grep "TOTEN" OUTCAR | tail -1 | awk '{printf "%12.6f\n",$5}'`
echo $i $E >> comment
done
```



# 三、截断能的测试和SIGMA测试

## SIGMA测试

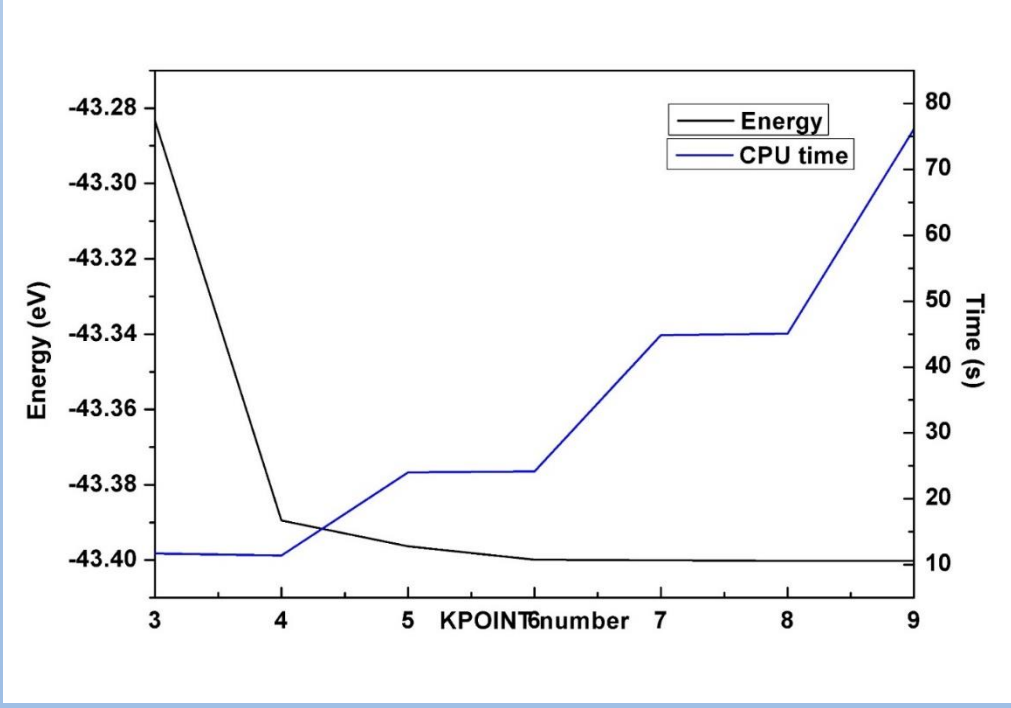
- 脚本

```
for i in 0.5 0.4 0.3 0.2 0.1 0.05 0.02 0.01
do
cat > INCAR <<!
SYSTEM = Rutile
SIGMA = $i
.....
!
echo "ENCUT= $i eV";
rm -f WAVECAR CHGCAR
run vasp
E=`grep "TOTEN" OUTCAR | tail -1 | awk '{printf "%12.6f\n",$5}'`
echo $i $E >> comment
done
```

# 四、K点测试

• 脚本

```
for i in 1 2 3 4 5 6 7 8 9
do
cat > KPOINTS <<!
auto
0
Gamma
$i $i $i
0. 0. 0.
!
echo "ENCUT= $i eV";
rm -f WAVECAR CHGCAR
run vasp
E=`grep "TOTEN" OUTCAR | tail -1 | awk '{printf "%12.6f\n",$5}'`
echo $i $E >> comment
done
```



# 影响计算效率的其它因素

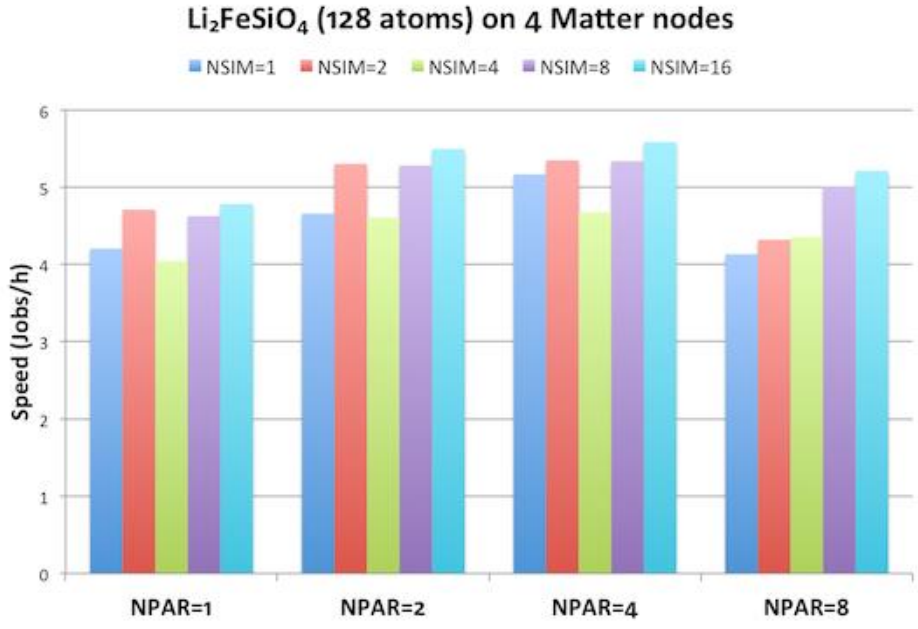
1、晶胞的大小

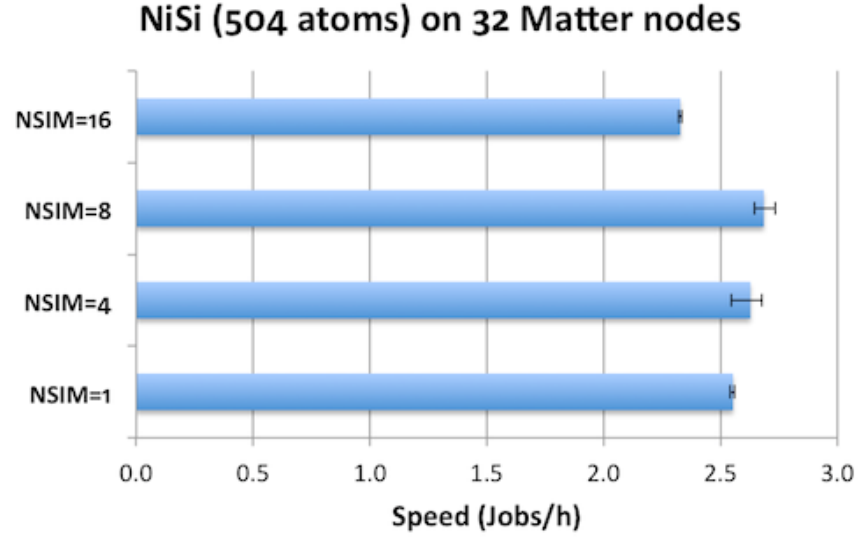
2、对称性 (ISYM)

3、并行计算参数NPAR、NSIM、KPAR等

In conclusion:

- Use NPAR = 1 and NSIM = 2 for single-node jobs
- Use NPAR = nodes/2 (or nodes) and NSIM=2 for medium jobs. If you have enough bands per core and want to optimize, you can try NSIM=8/16 and see if it helps.
- Use NPAR = sqrt(nodes) and NSIM=4 for large jobs.




https://www.nsc.liu.se/~pla/blog/2012/02/22/nparnsim/

# 如何解决收敛性问题

(关注学术之友微信公众号“加快磁性材料电子迭代收敛经验小结”文章)

**The ALGO tag is a convenient option to specify the electronic minimisation algorithm in VASP.4.5 and later versions.**

ALGO = Very_Fast (速度快，稳定性差)

ALGO = Normal (稳定性最好)

ALGO = Fast (结合了前面2种的优点)

ALGO = Damped (HSE06计算)

ALGO = All (HSE06计算)

ALGO = Exact (光学计算)

磁性体系还需要考虑：

MIXING参数(AMIX, BMIX)

ALGO = Exact performs an exact diagonalization (IALGO = 90), and we recommend to use this if more than 30-50 % of the states are calculated (e.g. for GW or RPA calculations).

# 第五讲 VASP结构优化

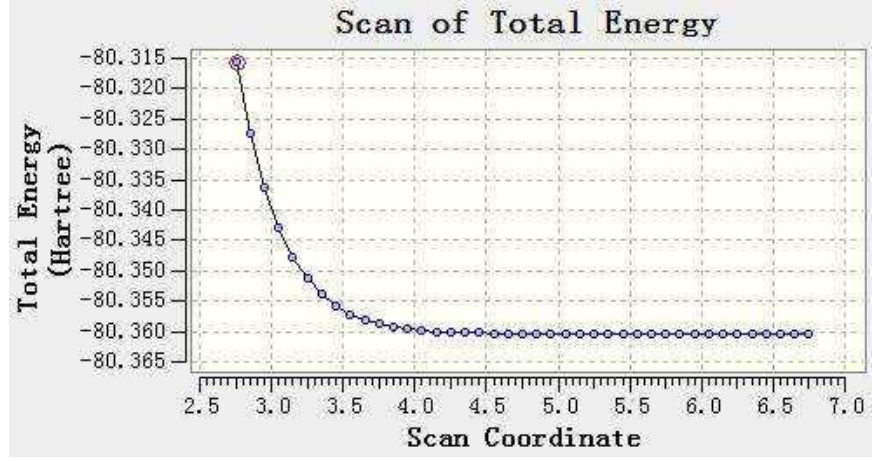
易文才

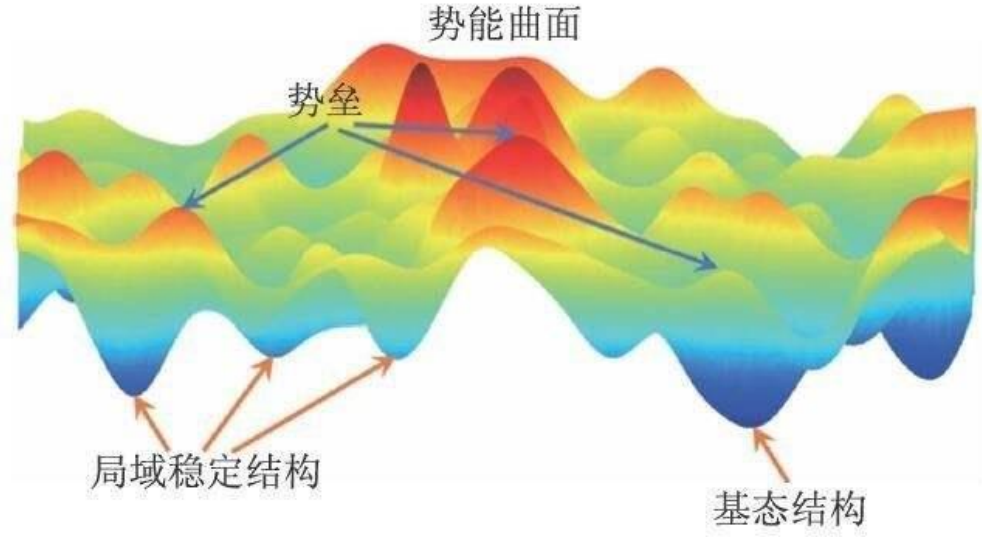
# 主要内容

一、原胞优化

二、表面优化

三、气体小分子和团簇优化



# 一、原胞优化

思考：为什么从实验得来的晶体结构需要做结构优化？
如何优化原胞？

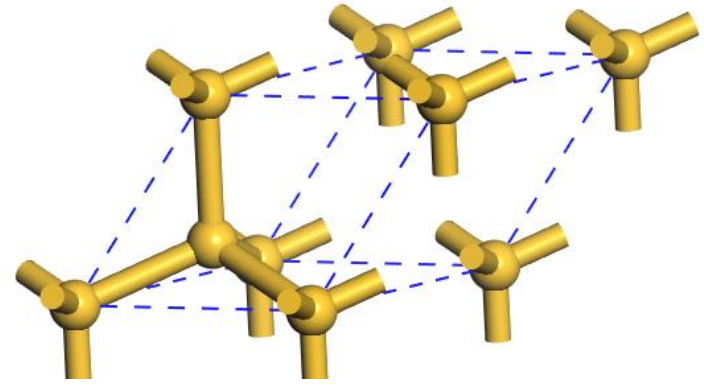
两种优化方法：

1、直接在INCAR中设置ISIF=3，优化原子位置的同时优化晶格参数。(直接法)

2. 保持晶格参数比例，对晶胞进行缩放，得到能量与缩放系数之间的关系图，取能量最低的点为最终结果。(间接法)

# 一、原胞优化(直接法)

INCAR
SYSTEM = Si; PREC = Normal; ENCUT = 500 eV ;
EDIFF = 1E-5; EDIFFG = -0.02; LREAL = F
LCHARG = F; LWAVE = F; GGA = PE
NSW = 300; IBRION = 2; ISIF = 3;



Si-bulk
1.0
3.8401000500 0.0000000000 0.0000000000
1.9200500250 3.3256241964 0.0000000000
1.9200500250 1.1085413988 3.1354285612
Si
2
Direct
0.000000000 0.000000000 0.000000000
0.250000000 0.250000000 0.250000000

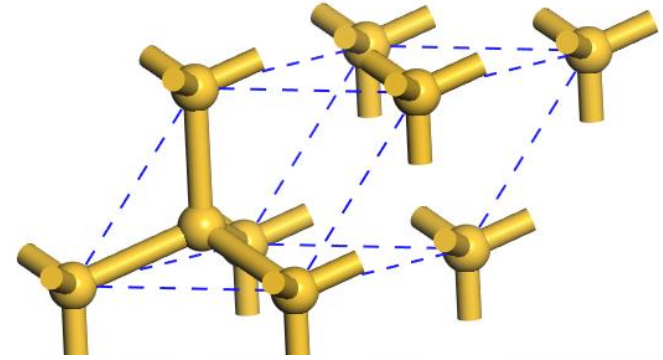
KPOINTS:
Auto
0
G
9 9 9
0. 0. 0.

# 一、原胞优化(直接法)

CONTCAR

Si-bulk
1.00000000000000
3.8668082709276259 0.0000000000000000 0.0000000000000000
1.9334041354638130 3.3487541942137558 -0.0000000000000000
1.9334041354638130 1.1162513980712518 3.1572357322691214
Si
2
Direct
0.0000000000000000 -0.0000000000000000 -0.0000000000000000
0.2500000000000000 0.2500000000000000 0.2500000000000000

晶格常数由3.8401变为3.8668
略微增大，属于正常情况



# 一、原胞优化(间接法)

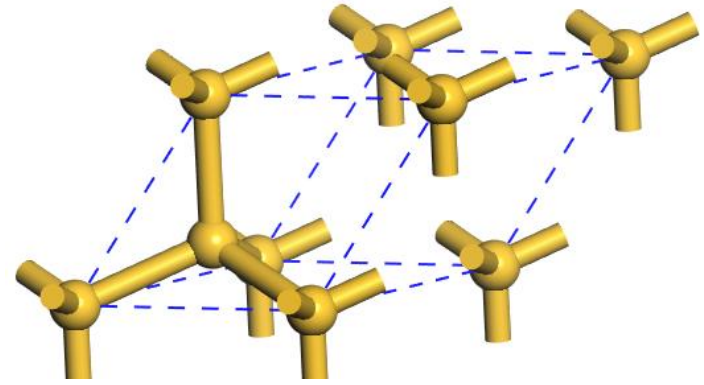
INCAR

SYSTEM = Si; PREC = Normal; ENCUT = 500 eV ;

EDIFF = 1E-5; EDIFFG = -0.02; LREAL = F

LCHARG = F; LWAVE = F; GGA = PE

NSW = 300; IBRION = 2; ISIF = 2;



Si-bulk

0.95-1.06 (用for循环控制)

```
      3.8401000500      0.0000000000      0.0000000000
      1.9200500250      3.3256241964      0.0000000000
      1.9200500250      1.1085413988      3.1354285612
   Si
    2
Direct
     0.000000000       0.000000000       0.000000000
     0.250000000       0.250000000       0.250000000
```

KPOINTS：

Auto

0

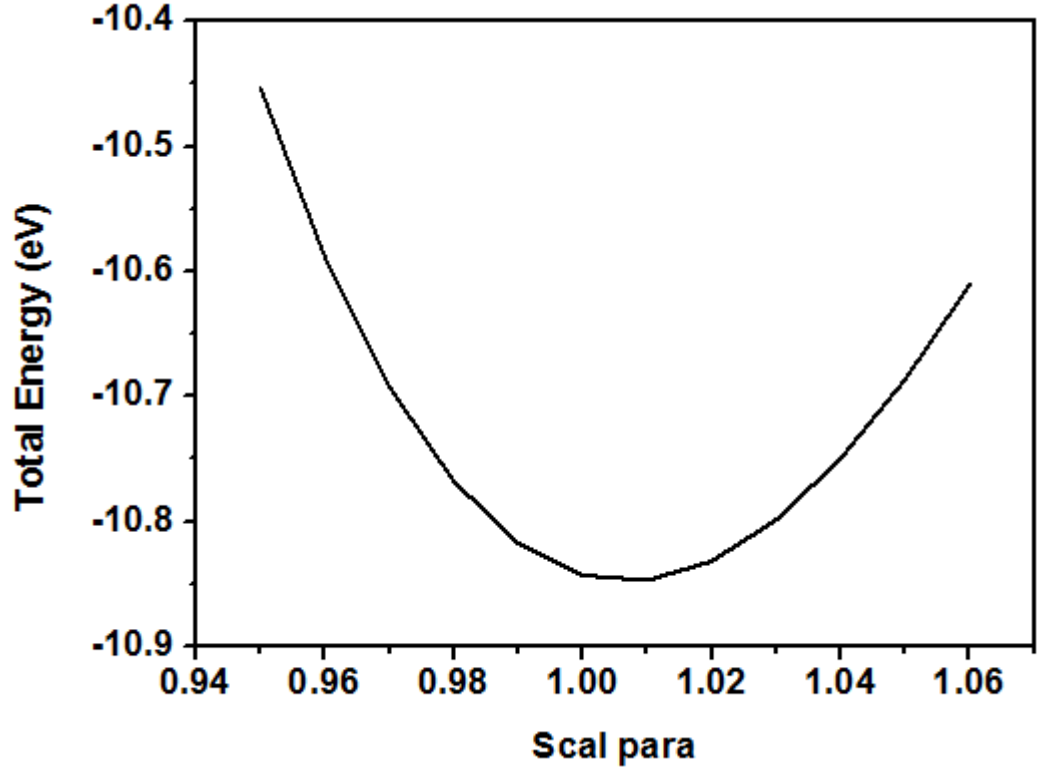
G

9 9 9

0. 0. 0.

# 一、原胞优化(间接法)

```
for i in 0.95 0.96 0.97 0.98 0.99 1.00 1.01 1.02 1.03 1.04 1.05 1.06
do
cat > POSCAR <<!
Si-bulk
$i
        3.8401000500          0.0000000000          0.0000000000
        1.9200500250          3.3256241964          0.0000000000
        1.9200500250          1.1085413988          3.1354285612
   Si
    2
Direct
     0.000000000          0.000000000          0.000000000
     0.250000000          0.250000000          0.250000000
!
mpirun -np $1  $EXEC > log
E=`grep "without entropy" OUTCAR |tail -n 1|awk '{printf $7}'`
cputime=`grep "CPU" OUTCAR |awk '{printf $6}'`
echo $i $E $cputime >> comment
mv CONTCAR CONTCAR-$i
mv OUTCAR OUTCAR-$i
done
```

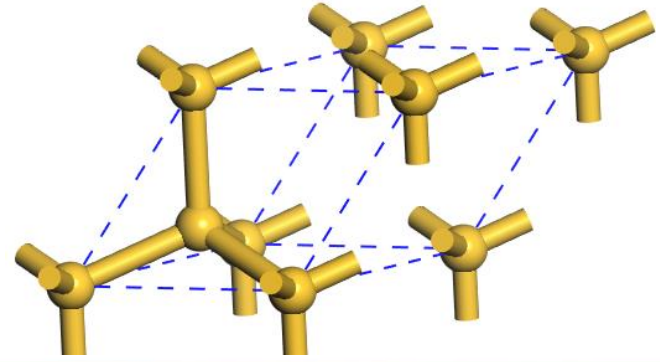



Scale=1.01

得到晶胞参数

a=b=c= 3.8401 *1.01Å=3.878501Å

比实验值大1.000%

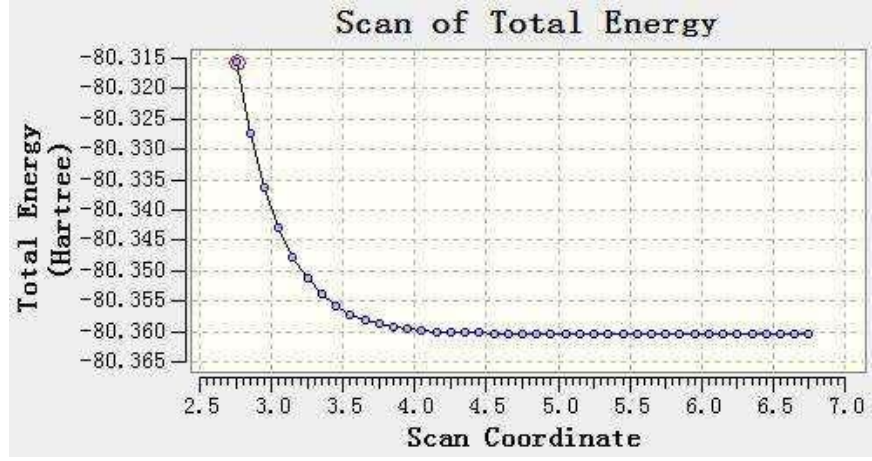


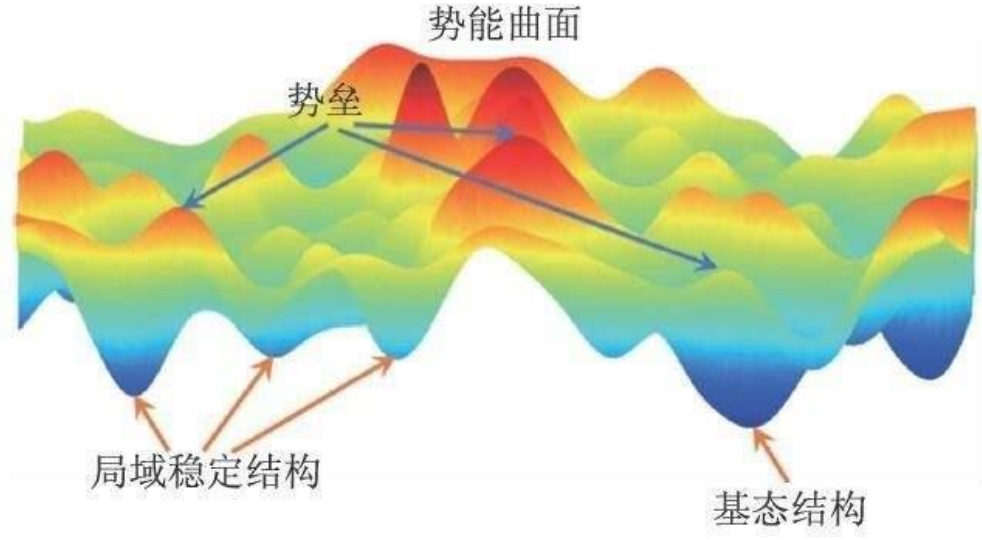
# 主要内容

一、原胞优化

二、表面优化

三、气体小分子和团簇优化



# 二、表面优化

INCAR

SYSTEM = Si; PREC = Normal; ENCUT = 500 eV ;

EDIFF = 1E-5; EDIFFG = -0.02; LREAL = F

LCHARG = F; LWAVE = F; GGA = PE

NSW = 300; IBRION = 2; ISIF = 2;

```
Cu-CHO
1.0
        5.1119999886          0.0000000000          0.0000000000
       -0.0000088492          5.1119999885          0.0000000000
       -0.0000266965         -0.0000266965         15.4221000671
   Cu    C    O    H
   16    1    1    1
Selective dynamics
Direct
     0.000030000          0.001330000          0.179790005    F    F    F
     0.000100000          0.005870000          0.410259992    T    T    T
     0.250000000          0.250000000          0.064839996    F    F    F
     0.255829990          0.251619995          0.299970001    T    T    T
     0.500010014          0.000420000          0.179309994    F    F    F
     0.500079989          0.003300000          0.420670003    T    T    T
     0.750000000          0.250000000          0.064839996    F    F    F
     0.744279981          0.251610011          0.299959987    T    T    T
     0.000020000          0.499980003          0.180910006    F    F    F
     0.000020000          0.502420008          0.413540006    T    T    T
     0.250000000          0.750000000          0.064839996    F    F    F
     0.253170013          0.752380013          0.299329996    T    T    T
     0.500020027          0.500800014          0.179820001    F    F    F
     0.500029981          0.493849993          0.421799988    T    T    T
     0.750000000          0.750000000          0.064839996    F    F    F
     0.746959984          0.752409995          0.299309999    T    T    T
     0.500989974          0.632679999          0.538280010    T    T    T
```

KPOINTS：

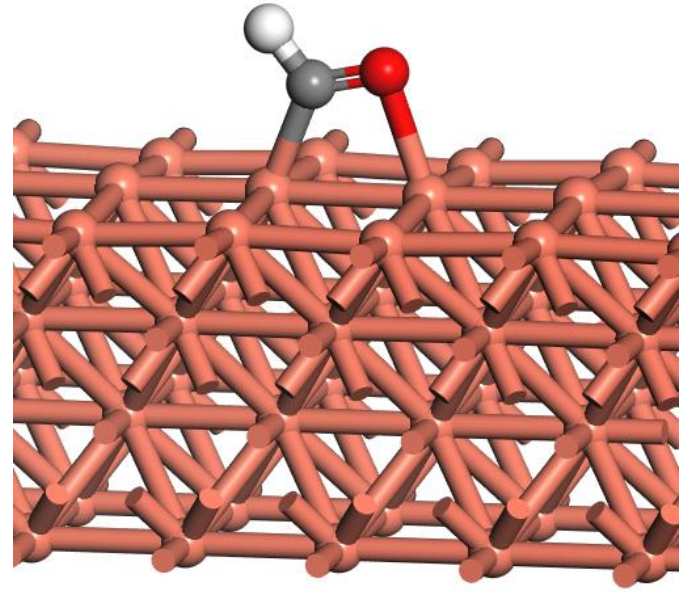
Auto

0

G

3 3 1

0. 0. 0.

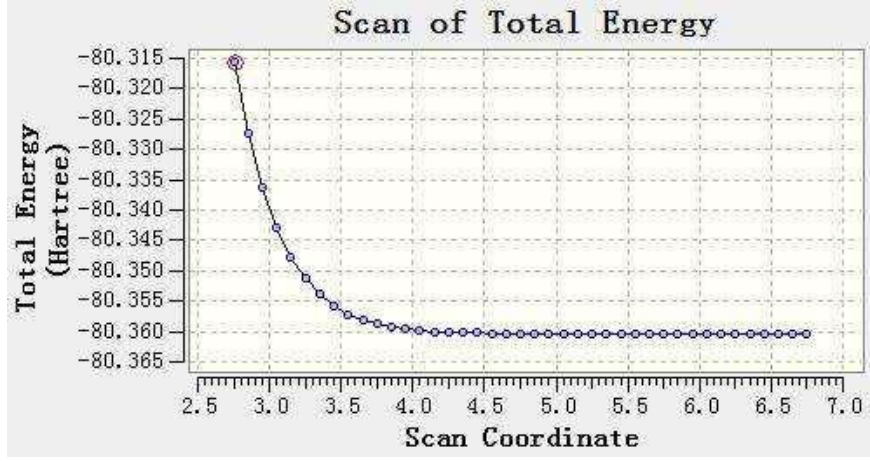


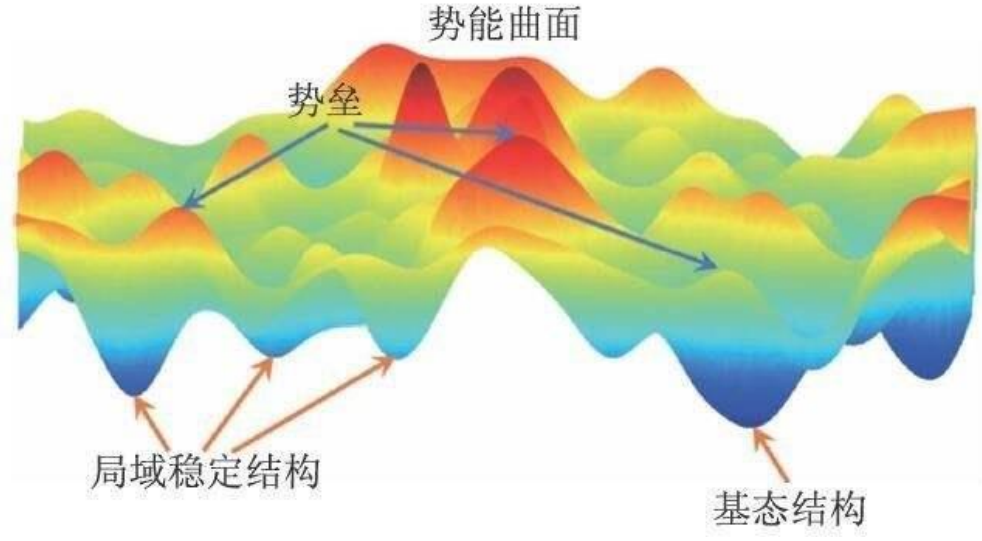
# 主要内容

一、原胞优化

二、表面优化

三、气体小分子和团簇优化



# 三、气体小分子和团簇优化

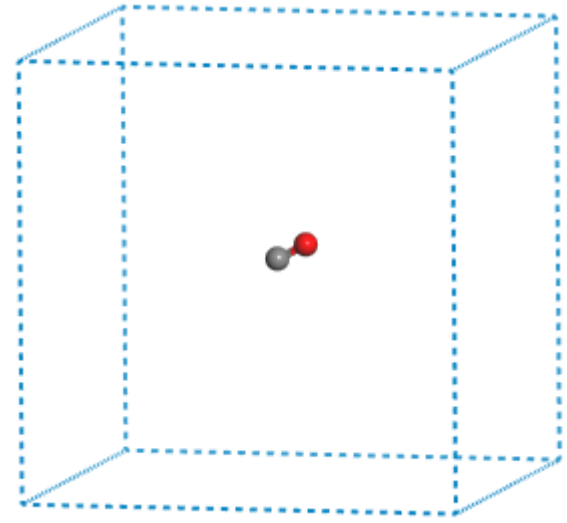
INCAR

SYSTEM = Si; PREC = Normal; ENCUT = 500 eV ;

EDIFF = 1E-5; EDIFFG = -0.02; LREAL = F

LCHARG = F; LWAVE = F; GGA = PE

NSW = 300; IBRION = 2; ISIF = 2;



CO

1.0

15.0000000000 0.0000000000 0.0000000000

0.0000000000 15.0000000000 0.0000000000

0.0000000000 0.0000000000 15.0000000000

C O

1 1

Direct

0.465659976 0.499310017 0.469669998

0.533050001 0.533720016 0.476460010

计算结果存于CONTCAR文件中，就不加以赘述了

KPOINTS：

Auto

0

G

1 1 1

0. 0. 0.

# 回顾、熟悉和提问

1、VASP优化原胞有几种方法？效果如何？如何检验是否优化到局域极小点了？

2、优化表面与优化原胞有什么不同？

3、优化气体小分子和团簇与优化原胞有什么不同？

4、二维材料原胞如何优化？

5、一维链状结构如何优化？