赝势、投影函数与 VASP 的 POTCAR

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球形势对平面波的散射与相移

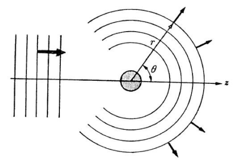

Fig.: Schematic illustration of scattering of a plane wave by a spherical potential.

入射平面波

$$e^{i\vec{q}\cdot\vec{r}} = 4\pi \sum_{lm} i^l j_l(\vec{q}\cdot\vec{r}) Y^*_{lm}(\hat{\vec{q}}) Y_{lm}(\hat{\vec{r}}) = \sum_l (2l+1) i^l j_l(qr) P_l(\cos\theta)$$

经散射后出射，波函数变为

$$\Psi_l^{>}(\varepsilon, r) = C_l \left[j_l(\kappa r) - \tan\eta_l(\varepsilon) n_l(\kappa r) \right] \quad \text{其中}\kappa^2 = \varepsilon$$

根据散射理论，能量为 ε 的电子经单个势阱散射偏转 θ 后，波函数的振幅可以表示为

$$t(\theta) = \frac{4\pi}{\kappa} \sum_l (2l+1)[\exp(2i\eta_l(\varepsilon)) - 1] P_l(\cos\theta)$$

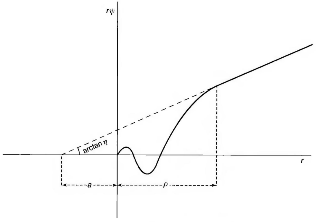

Fig.: Radial wave-function $\phi = r\psi$ for low-energy scattering as illustrated in a figure from the 1934 and 1935 papers of Fermi and coworkers for low-energy electron scattering from atoms and neutron scattering from nuclei. The node in the wave-function near the origin show that the potential is attractive and strong enough to have bound states. The cross-section for scattering from the localized potential is determined by the phase shift and is the same for weaker pseudo-potential with the same phase shift modulo 2π.

对于球形势散射，相移可由径向波函数计算

$$\tan\eta_l(\varepsilon) = \frac{R\frac{\mathrm{d}}{\mathrm{d}r}j_l(\kappa r)|_R - D_l(\varepsilon)j_l(\kappa R)}{R\frac{\mathrm{d}}{\mathrm{d}r}n_l(\kappa r)|_R - D_l(\varepsilon)n_l(\kappa R)}$$

$$\text{其中}\ D_l(\varepsilon, r) \equiv r\psi_l'(r)/\psi_l(r) = r\frac{\mathrm{d}}{\mathrm{d}r}\ln\psi_l(r)$$

同时相移与波函数节点的关系为:

$$\eta_l(\varepsilon) = p_l\pi + \delta(\varepsilon)$$

由 OPW 到赝势

赝势、投影函数与 VASP 的 POTCAR

赝势理论

平面波与赝势

模守恒赝势与超软赝势

可分离赝势与 Ghost band

VASP 中的 PAW 原子数据集

AtomPAW 赝势 Data set 的生成

- 完全平面波基组

  少数平面波就可以很好地描述波函数在原子间的行为，近核波函数则需要大量平面波展开

- 正交平面波 (Orthogonalized plane wave, OPW) 方法

  价电子波函数由芯电子波函数和平面波共同展开

$$\phi_{\mathrm{OPW}}^{\vec{k}+\vec{G}}(\vec{r}) = \phi_{\mathrm{PW}}^{\vec{k}+\vec{G}}(\vec{r}) - \sum_c \langle \varphi_c | \phi_{\mathrm{PW}}^{\vec{k}+\vec{G}} \rangle \varphi_c(\vec{r})$$

通过价电子和芯电荷波函数叠加构造赝波函数

$$\tilde{\phi}_v(\vec{r}) = \phi_v(\vec{r}) + \sum_c \langle \varphi_c | \tilde{\phi}_v \rangle \varphi_c(\vec{r})$$

代入 Schrödinger 方程

$$\hat{H}|\tilde{\phi}_v\rangle - \sum_c \langle \varphi_c | \tilde{\phi}_v \rangle \hat{H} |\varphi_c\rangle = \varepsilon_v |\tilde{\phi}_v\rangle - \varepsilon_v \sum_c \langle \varphi_c | \tilde{\phi}_v \rangle |\varphi_c\rangle$$

可有

$$\hat{H}|\tilde{\phi}_v\rangle + V^R |\tilde{\phi}_v\rangle = \varepsilon_v |\tilde{\phi}_v\rangle$$

这里排斥势是

$$V^R(\vec{r}, \vec{r}') = \sum (\varepsilon_v - \varepsilon_c) |\varphi_c(\vec{r}')\rangle \langle \varphi_c(\vec{r})|$$

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Phillips-Kleinman 指出，赝势 (V^{eff})-赝波函数 (可用 $\phi_{\mathrm{PW}}^{\vec{k}+\vec{G}}$ 展开) 满足 Schrödinger 方程

$$\left(-\frac{1}{2}\nabla^2+V^{\mathrm{eff}}\right)|\tilde{\phi}_v\rangle=\varepsilon_v|\tilde{\phi}_v\rangle$$

其中 $V^{\mathrm{eff}}=V(\vec{r})+V^R$

- 赝势-赝波函数的本征值 ε_v 与真实体系的价电子能量本征值相等
- 赝势 V^{eff} 比 $V(\vec{r})$ 平滑得多，并且 V^R 是非局域的排斥势

$$\begin{aligned}V^Rf(\vec{r})&=\sum_c(\varepsilon_v-\varepsilon_c)\varphi_c(\vec{r})\int\varphi_c^*(\vec{r}')f(\vec{r}')\mathrm{d}\vec{r}'\\&=\int V^R(\vec{r},\vec{r}')f(\vec{r}')\mathrm{d}\vec{r}'\end{aligned}$$

PK 型赝势

Phillips-Kleinman (PK) 赝势取为

$$\tilde{V}^{\rm PK}=V(\vec{r})+\sum_c(\varepsilon_v-\varepsilon_c)|\varphi_c\rangle\langle\varphi_c|$$

对应的赝波函数可以表示为

$$|\tilde{\psi}^{\rm PK}\rangle=|\psi_t\rangle-\sum_c\langle\varphi_c|\psi_t\rangle|\varphi_c\rangle$$

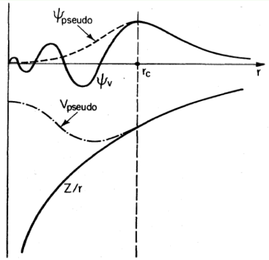
PK 型赝势的一些不足

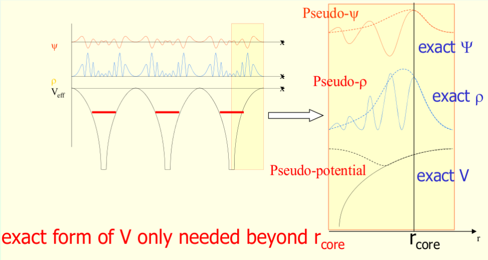
- 构造赝波函数时必须有与价电子正交的芯电子波函数:
  因此对于 $1s$、$2p$、$3d$ 等轨道，无法实施 PK 型赝化方案
- 赝势 $\tilde{V}^{\rm PK}$ 依赖于能量本征值 ε_v:
  源于正交平面波的非正交归一性，导致构建的久期方程的非对角元项对能量依赖
- 与芯电荷区以外，赝波函数与价波函数的模不相等:
  每次计算后必须将波函数重新归一化

赝势的评估

赝势 (Pseudo Potential, PP) 方法是在正交平面波的基础上发展起来的，构造出平缓的势函数代替核的强吸引作用和芯层电子的排斥作用，用平缓的函数取代波函数近核时的震荡。

- 赝势-平面波方法，只需要少量平面波可展开赝波函数，大大提升了计算效率；但是赝波函数不能很好地反映与电子近核行为有关的性质。
- 赝势的构造并不唯一，考核构造赝势的两大指标: “柔软程度”(Soft) 与 “可移植性”(transferability)





传统赝势的构造

直接由实验数据来确定 (模型) 赝势，常用的实验数据包括离子对电子的散射角度、离子的光谱实验数据等

- 构造离子赝势: 可移植性好
- 构造总赝势 (包括全部价电子相互作用): 常用于能带描述

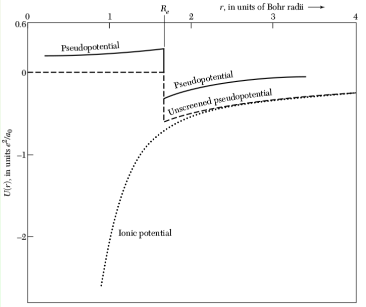


Fig.: Pseudopotential for metallic sodium, based on the empty core model and screened by the Thomas-Fermi dielectric function.

传统赝势的构造

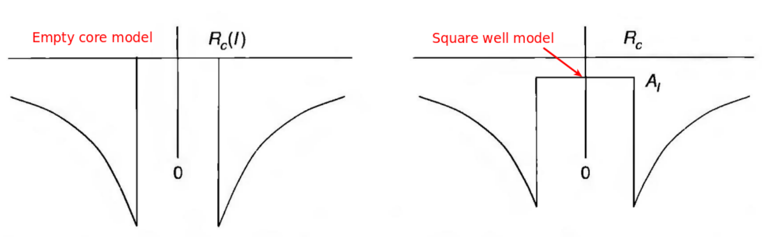


Fig.: Left:"Empty core" model potential of Ashcroft in which the potential is zero inside radius $R_c(l)$ which is different for each l. Right: Square well model potential with value A_l inside a cut-off radius R_c, proposed by Abarenkov and Heine and fit to atomic data by Animalu and Heine. The fact that the potential are weak, zero, or even positive inside cut-off radius R_c is an illustration of the "cancellation theorem".

由第一原理求解出全电子波函数 (径向部分)$P_{n,l}(r)$

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l(l+1)}{2r^2}+V(\rho,r)\right]P_{n,l}(r)=\varepsilon_{n,l}P_{n,l}(r)$$

这里 $V(\rho,r)$ 是自洽单电子势

$$V(\rho,r)=-\frac{Z}{r}+V_{\mathrm{H}}(\rho,r)+V_{XC}^{\mathrm{LDA}}(\rho(r))$$

$V_{\mathrm{H}}(\rho,r)$ 是 Hartree 势，$V_{XC}^{\mathrm{LDA}}(\rho(r))$ 是交换-相关势
由此构造赝波函数 $P_l^{\mathrm{PS}}(r)$，满足

$$P_l^{\mathrm{PS}}(r)=P_l^{\mathrm{AE}}(r),\quad r>r_{cl}$$

进而构造赝势 $V_{\mathrm{src},l}^{\mathrm{PP}}(r)$

$$V_{\mathrm{src},l}^{\mathrm{PP}}(r)=\varepsilon_l-\frac{l(l+2)}{2r^2}+\frac{1}{2P_l^{\mathrm{PS}}(r)}\frac{\mathrm{d}^2}{\mathrm{d}r^2}P_l^{\mathrm{AE}}(r),\quad r>r_{cl}$$

1. 价电子赝波函数的能量本征值与对应全电子波函数能量本征值相等: $\varepsilon_l^{\rm PP}=\varepsilon_l^{\rm AE}$
2. 价电子赝波函数与真实电子波函数的径向部分在截断半径 $r_{c,l}$ 外相同: $\psi_l^{\rm PP}(r)=\psi_l^{\rm AE}(r),\quad r>r_{cl}$
3. 价电子赝波函数与真实电子波函数的对数导数在截断半径 $r_{c,l}$ 处相等: $D_l^{\rm PP}(r)=D_l^{\rm AE}(r),\quad r\geqslant r_{cl}$(可移植性基础)

   这里 $D_l(\varepsilon,r)=r\frac{\psi_l'(\varepsilon,r)}{\psi_l(\varepsilon,r)}=r\frac{\mathrm{d}}{\mathrm{d}r}\ln\psi_l(\varepsilon,r)$
4. 价电子赝波函数与真实电子波函数在截断半径 $r_{c,l}$ 内的积分电荷相等 (模守恒条件)

$$Q_l=\int_0^{r_{cl}}\mathrm{d}r r^2|\psi_l^{\rm PP}(r)|^2=\int_0^{r_{cl}}\mathrm{d}r r^2|\psi_l^{\rm AE}(r)|^2$$

5. 价电子赝波函数与真实电子波函数的对数导数一阶能量导数 $\mathrm{d}D_l(\varepsilon,r)/\mathrm{d}\varepsilon$ 在截断半径 $r_{c,l}$ 处及以外相等 (强化可移植性)

模守恒 (Norm-conserving) 条件

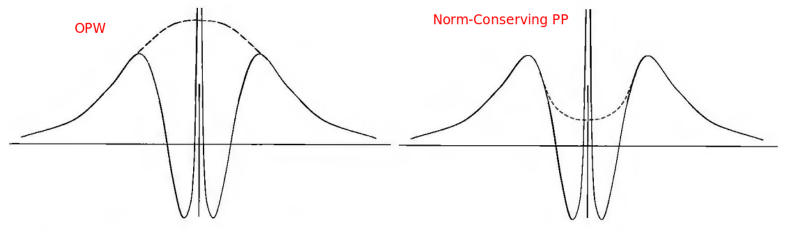


Fig.: Schematic example of a valence function that has the character of a 3*s* orbital near the nucleus and two examples of smooth functions (dashed lines) that equal the full wave-function outside the core region. Left: the smooth part of the valence function defined by OPW-like equation; Right: a smooth pseudo-function that satisfies the norm-conservation condition.

由原子赝波函数 (径向部分) 构造赝势类似于求解类 H 原子波函数
赝原子波函数的径向部分是轨道角动量依赖的

$$\psi_l^{\mathrm{PS}}(r) = r\phi_l^{\mathrm{PS}}(r)$$

因此得到赝势函数 (径向部分)$V_l(r)$ 也是角动量依赖的
为提高赝势的可移植性，减少构造赝势对环境的依赖，需要对其进行 “去屏蔽”

$$V_l(r) \equiv V_{l,src}^{\mathrm{PP}} - V_{\mathrm{Hartree}}^{\mathrm{PP}}(r) + V_{\mathrm{XC}^{PP}}(r)$$

实际应用时习惯将赝势 (径向部分) 分解为局域部分 (与角动量 l 无关)和非局域部分

$$V_l(r) = V_{\mathrm{local}}(r) + \delta V_l(\vec{r})$$

考虑角度部分后，角动量 l 相关的赝势 δV_l 将是半局域

$$V_{\mathrm{SL}} = V_{\mathrm{local}}(r) + \sum_{lm} |Y_{lm}\rangle \delta V_l \langle Y_{lm}|$$

角动量 l 相关赝势

赝势是在原子 (或离子) 条件下构造的，它依赖于能量 ε_l 的选择

$$V_l(r,\varepsilon_l) = V_{\text{local}}(r) + \delta V_l(r,\varepsilon_l)$$

在原子、分子构型下，一般取无穷远为势能零点: $\varepsilon < 0$

- 在无限扩展的周期体系中，势能平均值 (能量的参考零点) 是无法确定的
  构造第一原理赝势时，需要考虑参数 ε_l 的值无法唯一确定带来的影响
- 构造 PK 型赝势时，能量参数为 $\varepsilon_v - \varepsilon_c$:
  能量差不依赖周期体系势能的平移常数，不存在上述问题

角动量 l 相关赝势计算的困难与克服

半局域型赝势在用平面波展开时，需要计算大量 ($\vec{k}$ 和 $\vec{k}'$ 都相关) 的积分项

$$\int j_l(k\cdot r)V_l(r)j_l(k'\cdot r)r^2\mathrm{d}r P_l(\cos\theta_{kk'})$$

这里 j_l 是球 Bessel 函数
$P_l(\cos\theta_{kk'})$ 是矢量 $\vec{k}$ 和 $\vec{k}'$ 夹角的 Legendre 多项式函数

Kleinman-Bylander 等注意到: 如果角动量 l 相关的半局域型赝势可写成类似 PK 型赝势的形式，则平面波展开可写成

$$\int j_l(k\cdot r)\varphi_l^c(r)(r)r^2\mathrm{d}r\int j_l(k'\cdot r')\varphi_l^c(r')r'^2\mathrm{d}r' P_l(\cos\theta_{kk'})$$

显然，大量积分将以乘积形式出现，因此需要独立计算的积分 (仅与 $\vec{k}$ 相关) 数量将大大减少

非局域赝势的变量分离

Kleinman-Bylander 仿照 PK 型赝势的特点，提出了非局域赝势的变量分离方案[1]:
如果选择适当的局域函数 $V^{\mathrm{PP}}_{\mathrm{local}}(r)$，赝势将可分解为局域部分与非局域部分之和 (这种分解称为 factored pseudo-potential)

$$\hat{V}^{\mathrm{PP}}_{\mathrm{NL}}(r)=V^{\mathrm{PP}}_{\mathrm{local}}(r)+\sum_{lm}\frac{|\psi^{\mathrm{PS}}_{lm}\delta V_l\rangle\langle\delta V_l\psi^{\mathrm{PS}}_{lm}|}{\langle\psi^{\mathrm{PS}}_{lm}|\delta V_l|\psi^{\mathrm{PS}}_{lm}\rangle}$$

这是将 δV_l 表示到 ψ^{PS}_{lm} 构成的空间中，$\langle\delta V_l(r)\psi^{\mathrm{PP}}_{lm}|$ 是投影子

$$\langle\delta V_l\psi^{\mathrm{PS}}_{lm}|\psi\rangle=\int \mathrm{d}\vec{r}\delta V_l(r)\psi^{\mathrm{PS}}_{lm}(\vec{r})\psi(\vec{r})$$

投影函数局域在截断半径内，该区域内 δV_l 有非零值

- 投影函数的存在，保证了即使非束缚态也可以作为赝波函数

[1] 即 $\delta V(\vec{r},\vec{r}')$ 可以写成 $\delta V(\vec{r},\vec{r}')=\sum_i f_i(\vec{r})g_i(\vec{r}')$ 的形式

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应用投影函数，非局域赝势矩阵元的计算也变得更方便

$$\langle\psi_i|\delta V_{\mathrm{NL}}|\psi_j\rangle=\sum_{lm}\langle\psi_i|\psi_{lm}^{\mathrm{PS}}\delta V_l\rangle\frac{1}{\langle\psi_{lm}^{\mathrm{PS}}|\delta V_l|\psi_{lm}^{\mathrm{PS}}\rangle}\langle\delta V_l\psi_{lm}^{\mathrm{PS}}|\psi_j\rangle$$

更一般地，如果允许赝势局域部分 $V_{\mathrm{local}}^{\mathrm{PP}}(r)$ 为任意函数，则可定义辅助函数

$$\chi_{lm}^{\mathrm{PS}}(\vec{r})=\left\{\varepsilon_l-\left[-\frac{1}{2}\nabla^2+V_{\mathrm{local}}^{\mathrm{PP}}(\vec{r})\right]\right\}\psi_{lm}^{\mathrm{PS}}(\vec{r})$$

于是赝势的非局域部分可表示为

$$\delta V_{\mathrm{NL}}=\sum_{lm}\frac{|\chi_{lm}^{\mathrm{PS}}\rangle\langle\chi_{lm}^{\mathrm{PS}}|}{\langle\chi_{lm}^{\mathrm{PS}}|\psi_{lm}^{\mathrm{PS}}\rangle}$$

但是 $V_{\mathrm{local}}^{\mathrm{PP}}(r)$ 选择的随意性，将增加计算结果出现 Ghost band 的风险

Ghost band 的表现

只有价电子的赝波函数与芯电子波函数完全正交，能带计算中才能确保芯层与价层电子的完全分离。但实际计算时，该正交条件很难严格保证，因此一旦赝波函数严重偏离正交条件，计算的能带中会在本不存在能带的区域出现电子结构分布 (称为 Ghost band)，这部分电子结构源自构造赝波函数的能量参数 ε_l 与芯层电子能量差别太大，无法保持与芯层电荷严格正交引起的

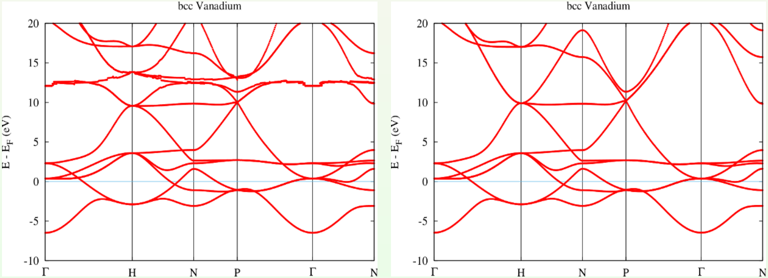

Fig.: The band structure of bcc Vanadium.
Left: Between 10 and 15 eV above the Fermi energy a strange band with nearly no dispersion can be observed. The vanishing dispersion of the band is a typical property of ghost bands.

Ghost band 的根源

可分离赝势方法中

$$\hat{\mathbf{H}} = -\frac{1}{2}\nabla^2 + V_{\text{local}}(r) + \delta\hat{V}_{\text{NL}}$$

赝波函数 $\psi_{lm}^{\text{PP}}(r)$ 是方程

$$\hat{\mathbf{H}}\psi_{lm}^{\text{PP}}(r) = \varepsilon_l \psi_{lm}^{\text{PP}}(r)$$

的解。

因为 $V_{\text{local}}(r)$ 可随意选择，因此赝波函数 $\psi_{lm}^{\text{PP}}(r)$ 和能量 ε_l 不再要求与束缚态波函数相对应，将导致 Ghost band 的出现

Ghost band 根源的数学说明 *

对于半局域势，求解能量 ε 对应的径向波函数 $u_l(r,\varepsilon)$ 的方程是一个常微分方程

$$-\frac{1}{2}\frac{\mathrm{d}^2 u_l}{\mathrm{d}r^2}+\overline{V}_l^{\mathrm{loc}}(r)u_l(r,\varepsilon)+\Delta V_l^{\mathrm{SL}}(r)u_l(r,\varepsilon)-\varepsilon u_l(r,\varepsilon)=0$$

而对于可分离赝势 (如 KB 势)，方程则为积分-微分方程

$$-\frac{1}{2}\frac{\mathrm{d}^2 u_l}{\mathrm{d}r^2}+\overline{V}_l^{\mathrm{loc}}(r)u_l(r,\varepsilon)+\int\Delta V_l(r,r')u_l(r',\varepsilon)\mathrm{d}r'-\varepsilon u_l(r,\varepsilon)=0$$

将可分离赝势代入可有

$$-\frac{1}{2}\frac{\mathrm{d}^2 u_l}{\mathrm{d}r^2}+\overline{V}_l^{\mathrm{loc}}(r)u_l(r,\varepsilon)+f_l(r)\int g_l(r')u_l(r',\varepsilon)\mathrm{d}r'-\varepsilon u_l(r,\varepsilon)=0$$

- 常微分方程解的结构服从 Wronskian 定理的推论: 本征态能量 $\varepsilon_0,\varepsilon_1,\cdots,\varepsilon_n$ 按升序排列时，对应的本征态波函数 (径向) 的节点数依次递增
- 积分-微分方程解的结构不要求满足该结论: 波函数的节点数与能量本征态不再有对应的升序关系

由于积分项的存在，传统的常微分方程求解算法 (如 Runger-Kutta 法等) 无法直接用于该积分-微分方程，必须另图别策

基本思想: 类似积分方程求解的 Fredholm 方法

- 先将微分方程中的积分项近似为常数因子，求解非齐次常微分方程
- 对含有波函数的积分，应用闭路积分公式 (closure formula) 计算

具体求解流程

1. 采用通用方法分别求解
齐次微分方程

$$-\frac{1}{2}\frac{\mathrm{d}^2W_l}{\mathrm{d}r^2}+\overline{V}_l^{\mathrm{loc}}(r)W_l(r,\varepsilon)-\varepsilon W_l(r,\varepsilon)=0$$

的通解和
不含积分项的非齐次微分方程

$$-\frac{1}{2}\frac{\mathrm{d}^2X_l}{\mathrm{d}r^2}+\overline{V}_l^{\mathrm{loc}}(r)X_l(r,\varepsilon)-\varepsilon X_l(r,\varepsilon)=f_l(r)$$

的一个特解

2. 构造积分

$$\tilde{W}(\varepsilon)=\int g_l(r)W(r,\varepsilon)\mathrm{d}r$$

$$\tilde{X}(\varepsilon)=1+\int g_l(r)X(r,\varepsilon)\mathrm{d}r$$

3. 由此得到积分-微分方程的解

$$u(r,\varepsilon)=K[W(r,\varepsilon)\tilde{X}(\varepsilon)-X(r,\varepsilon)\tilde{W}(\varepsilon)]$$

这里 K 是归一化因子

Ghost band 的克服

根据微分方程理论

$$\hat{\mathbf{H}}\psi_{lm}^{\mathrm{PP}}(r)=\varepsilon_l\psi_{lm}^{\mathrm{PP}}(r)$$

的解 $\psi_{lm}^{\mathrm{PP}}(r)$ 可表示为 (只考虑径向部分)

$$\psi_l^{\mathrm{PP}}(r)=u_l^0(r)+\sum_i c_i u_l^i(r)$$

这里 $u_l^0(r)$ 和 $u_l^i(r)$ 分别是齐次微分方程

$$\Big(-\frac{1}{2}\nabla^2+V_{\mathrm{local}}-\varepsilon_l^0\Big)u_l^0(r)=0$$

和非齐次微分方程

$$\Big(-\frac{1}{2}\nabla^2+V_{\mathrm{local}}-\varepsilon_l^j\Big)u_l^j(r)=\chi_l^j(r)$$

的解

引入多个能量参数 ε_l^i，通过优化控制参数 c_i，可以得到理想的局域势函数 $V_{\mathrm{local}}(r)$

为提高模守恒赝势的可移植性[2]，Vanderbilt 和 Blöchl 分别建议：在构造可分离赝势时，引入额外的参考能量 ε_l，并要求对每个角动量量子数 l，所有能量参数 ε_l 构造的赝波函数 $\phi_i^{\rm ps}$ 及其辅助函数 χ_i 都满足

$$|\chi_i\rangle = -(\mathbf{T} + V_{\rm loc} - \varepsilon)|\phi_i^{\rm ps}\rangle$$

这里 i 表示量子数 l，m 和能量参数 ε，即 $i = (lm, \varepsilon)$

由此出发，可构造出一组与赝波函数 $\phi_i^{\rm ps}$ 垂直的函数 β_i:

- 构造矩阵 $\mathbf{B}$，其矩阵元 B_{ij} 满足

$$B_{ij} = \langle\phi_j^{\rm ps}|\chi_i\rangle$$

- 由矩阵 $\mathbf{B}$ 和 χ 得到函数 β_i

$$|\beta_i\rangle = \sum_j (\mathbf{B}^{-1})_{ij}|\chi_j\rangle$$

- 由此得到的 β 与赝波函数 $\phi_i^{\rm ps}$ 满足正交条件

$$\langle\beta_i|\phi_j^{\rm ps}\rangle = \delta_{ij}$$

[2]换言之，提升赝波函数能适应的能量变分空间

因此可分离赝势的非局域部分表示为

$$V_{\mathrm{NL}} = \sum_i |\chi_i\rangle\langle\beta_i| = \sum_{ij} B_{ij}|\beta_j\rangle\langle\beta_i|$$

不难看出，如果赝波函数满足广义模守恒条件

$$Q_{ij} = \langle\phi_j^{\mathrm{AE}}|\phi_i^{\mathrm{AE}}\rangle - \langle\phi_j^{\mathrm{PS}}|\phi_i^{\mathrm{PS}}\rangle = 0$$

亦即

$$Q_{l\varepsilon,l\varepsilon'} = \int_0^{R_c}\left(\phi_{l\varepsilon}^{\mathrm{AE}}(r)\phi_{l\epsilon'}^{\mathrm{AE}}(r) - \phi_{l\varepsilon}^{\mathrm{PS}}(r)\phi_{l\varepsilon'}^{\mathrm{PS}}(r)\right)\mathrm{d}r = 0$$

将大大提高赝势的可移植性。

但实际上，广义模守恒条件看似简单，当能量参数 $\varepsilon \neq \varepsilon'$，要满足这个条件

$$Q_{l\varepsilon,l\varepsilon'} = 0$$

并非易事; 而一旦模守恒条件被破坏，矩阵 B(相应地，赝势的非局域部分 V_{NL}) 就是非 Hermitian

超软赝势

- 赝势构造的模守恒条件很好地解决了赝势可移植性问题，但对 $1s$、$2p$、$3d$ 等轨道，模守恒方案构造的赝势过于“硬”，所需平面波基组依然非常大
- 超软 (Ultra-soft) 赝势，解除模守恒条件，实现对第一、第二周期元素的高效计算

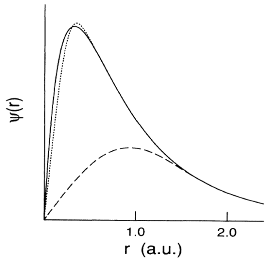

Fig.: Oxygen 2 p radical wave function (solid), NC-pseudo-wave (dotted) and US-pseudo-wave (dashed).

从模守恒赝势到超软赝势

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赝势、投影函数与 VASP 的 POTCAR

赝势理论
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VASP 中的 PAW 原子数据集

AtomPAW 赝势 Data set 的生成

Vanderbilt 建议构造赝波函数时放弃模守恒约束条件，只要求价电子赝波函数与真实电子波函数的径向部分在截断半径 $r_{c,l}$ 外相同，由此得到的赝势显然非 Hermitian，但是通过构造 Hermitian 重叠算符

$$\mathbf{S} = \mathbf{1} + \sum_{i,j} Q_{ij}|\beta_j\rangle\langle\beta_i|$$

以及Hermitian 赝势算符

$$\tilde{V}^{\mathrm{NL}} = \sum_{i,j} \mathbf{D}_{i,j}|\beta_j\rangle\langle\beta_i|$$

这里

$$\mathbf{D}_{ij} = B_{ij} + \varepsilon_i Q_{ij}$$

模守恒约束下的标准本征值方程将变成广义本征值方程

$$(T + V_{\mathrm{loc}} + \tilde{V}^{\mathrm{NL}} - \varepsilon\mathbf{S})|\phi\rangle = 0$$

超软赝势的特点

Vanderbilt 的超软赝势构造方案最大的优点是

- 解除模守恒约束: 有助于增加赝波函数的截断半径，系统提高赝势的柔软程度
- 引入多个参考能量 ε_l: 使得模守恒条件下只在特定参考能量 ε 处成立的对数导数连续条件，扩展到参考能量 ε_l 区间范围内，这大大提高了赝势的适用范围 (可移植性)

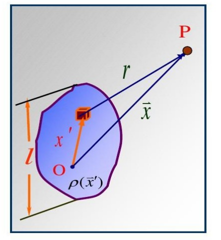
相应的，超软赝势计算中，电子密度表达形式为

$$n(r) = \sum_n f_n|\phi_n(r)|^2 + \sum_{n,ij} f_n\langle\phi_n|\beta_j\rangle\langle\beta_i|\phi_n\rangle Q_{ij}(r)$$

这里补偿电荷 $Q_{ij}(r)$ 定义为

$$Q_{ij}(r) = \phi_i^{\mathrm{AE}}(r)\phi_j^{\mathrm{AE}}(r)^* - \phi_i^{\mathrm{US}}(r)\phi_j^{\mathrm{US}}(r)^*$$

根据电动力学定理:
如果球 S 内的电荷密度分布 $\rho(\vec{r})$，在球外某点 $\vec{r}$ 产生的势是由电荷密度的多极矩确定:



$$V(\vec{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}q_{lm}\frac{Y_{lm}(\hat{\vec{r}})}{r^{l+1}}$$

其中多极矩 q_{lm} 由下式计算

$$q_{lm} = \int_S Y^*_{lm}(\hat{\vec{r}})r^l\rho(\vec{r})\mathrm{d}^3r$$

PAW Augmentation

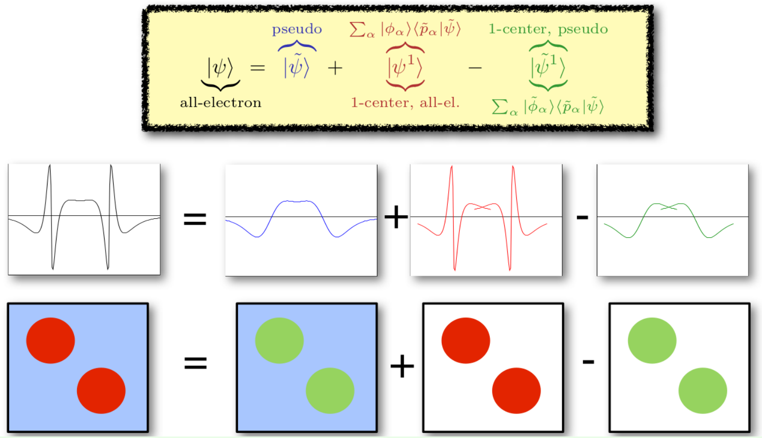


Fig.: The Augmentation of PAW.

平滑赝原子分波函数

$$\tilde{\phi}_{i=Lk}(\vec{r}) = Y_L(\widehat{\vec{r}-\vec{R}})\tilde{\phi}_{lk}(|\vec{r}-\vec{R}|)$$

根据 RRKJ 赝势构造，赝分波函数由球 Bessel 函数线性组合

$$\tilde{\phi}_{lk}(r) = \begin{cases} \sum_{i=1}^{2} \alpha_i j_l(q_i r) & r < r_c^l \\ \phi_{lk}(r) & r > r_c^l \end{cases}$$

调节系数 α_i 和 q_i 赝分波函数 $\phi_{lk}(r)$ 在截断半径 r_c^l 处两阶连续可微投影子波函数 $\tilde{p}_i$ 由 Gram-Schmidt 正交条件 $\langle\tilde{p}_i|\tilde{\phi}_j\rangle = \delta_{ij}$ 确定

VASP 中的 PAW 原子数据集

构造原子局域赝势 $\tilde{v}^a_{\text{eff}}$(为防止 ghost band):
在截断半径 r_{loc} 内的定义为

$$\tilde{v}^a_{\text{eff}} = A\frac{\sin(q_{loc}r)}{r} \quad r < r_{loc}$$

其中 q_{loc} 和 A 要求局域赝势在截断半径 r_{loc} 处连续到一阶导数
构造赝芯电荷密度 $\tilde{n}_c$: 在截断半径 r_{pc} 内的定义为

$$\sum_{i=1,2} B_i\frac{\sin(q_i r)}{r} \quad r < r_{pc}$$

调节系数 q_i 和 B_i 使得赝芯电荷密度 $\tilde{n}_c(r)$ 在截断半径 r_{pc} 处的两阶导数连续
局域离子赝势 $v_H[\tilde{n}_{Zc}]$ 可由原子局域赝势去屏蔽得到

$$v_H[\tilde{n}_{Zc}] = \tilde{v}^a_{\text{eff}} - v_H[\tilde{n}^1_a + \hat{n}_a] - v_{\text{XC}}[\tilde{n}^1_a + \hat{n}_a + \tilde{n}_c]$$

在 VASP 的 POTCAR 生成过程中，各截断半径的确定条件
$r_{rad} = \max(r^l_c)$,$r_{pc} \approx r_{rad}/1.2$,$r_{loc} < r_{rad}/1.2$

在每个原子球内用球 Bessel 函数构造补偿电荷 $g_l(r)$

$$g_l(r) = \sum_{i=1}^{2} \alpha_i^l j_l(q_i^l r)$$

调节系数 q_i^l 和 α_i^l 使得补偿电荷 $g_l(r)$ 在截断半径 r_{comp} 处的数值和前两阶导数值都是 0，因此可以选择 q_i^l 使得多极矩

$$\int_0^{r_{comp}} g_l(r) r^{l+2} \mathrm{d}r = 1$$

并且有

$$\left. \frac{\mathrm{d}}{\mathrm{d}r} j_l(q_i^l r) \right|_{r_{comp}} = 0$$

设置 α_i^l，因此 $g_l(r_{comp}) = 0$，$r_{comp} = r_{rad}/1.3 \sim r_{rad}/1.2$

几种赝势方法的关系

Pseudo-potential	Norm-Conservation PP		Ultra-Soft PP	PAW
		Separated PP		
Basis set	$\{e^{i\vec{k}\cdot\vec{r}}\}$	$\{e^{i\vec{k}\cdot\vec{r}}\}$	$\{e^{i\vec{k}\cdot\vec{r}}\}$	$\{e^{i\vec{k}\cdot\vec{r}},\phi_i(\vec{r}),\tilde{\phi}_i(\vec{r})\}$
Projector	-	$\{\tilde{\chi}_i(\vec{r})\}$	$\{\tilde{\beta}_i(\vec{r})\}$	$\{\tilde{p}_i(\vec{r})\}$
Charge	$\tilde{n}(\vec{r})$		$\tilde{n}(\vec{r}),\hat{n}(\vec{r})$	$\tilde{n}(\vec{r}),n^1(\vec{r}),\tilde{n}^1(\vec{r}),\hat{n}(\vec{r})$
Ion-Potential	$\tilde{V}_l^{\mathrm{loc}}(\vec{r}) + \sum_{l'}\sum_{m'} \lvert Y_{lm}\rangle V_{ll'}\langle Y_{l'm'}\rvert$	$\tilde{V}_l^{\mathrm{loc}}(r) + \sum_{l'} \lvert\tilde{\chi}_l(\vec{r})\rangle V_{ll'}\langle\tilde{\chi}_{l'}(\vec{r}')\rvert$	$\tilde{V}_l^{\mathrm{loc}}(r) + \sum_{l'} \lvert\tilde{\beta}_l(\vec{r})\rangle D_{ll'}\langle\tilde{\beta}_{l'}(\vec{r}')\rvert$	$\tilde{V}_l^{\mathrm{loc}}(r) + \sum_{l'} \lvert\tilde{p}_l(\vec{r})\rangle(D^1_{ll'} - \tilde{D}^1_{ll'} + \hat{D}_{ll'})\langle\tilde{p}_{l'}(\vec{r}')\rvert$

Fig.: The relation of Pseudo potential and PAW.

AtomPAW 程序的赝势构造

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求解原子的价层的全电子分波函数

$$\left(-\frac{\hbar^2}{2m}\nabla^2-\frac{Ze^2}{r}+e^2\int \mathrm{d}^3r'\frac{n_{core}(r')+n(r')}{|r-r'|}+\mu_{XC}[n_{core}(r)+n(r)]\right)|\phi_i\rangle=\epsilon_i|\phi_i\rangle$$

全电子分波电荷密度

$$n(r)=\sum_{n,l}c_{n,l}\frac{|\phi_{n,l}(r)|^2}{4\pi r^2}$$

有效赝势的构造方案

- Troullier-Martin NC 方案
  首先通过指数多项式构造赝波函数，要求满足

$$\tilde{\phi}(r) = \begin{cases} r^{L_v+1} e^{p(r)} & \text{for} \quad r \leqslant r_c \\ \phi(r) & \text{for} \quad r > r_c \end{cases}$$

这里

$$p(r) = \sum_{m=0}^{6} C_m r^{2m}$$

可得赝势

$$V_{\text{eff}}^{PS}(r) = \epsilon_l + \frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2 p}{\mathrm{d}r^2} + (\frac{\mathrm{d}p}{\mathrm{d}r})^2 + \frac{2(L_v+1)}{r}\frac{\mathrm{d}p}{\mathrm{d}r}\right)$$

于是赝 Hamiltonian 是 $\tilde{H}(r) = -\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}^{PS}(r)$

AtomPAW 程序的赝势构造

有效赝势的构造方案

- Ultra-soft 方案
  首先用多项式构造赝波函数，要求满足

$$\tilde{\phi}(r) = \begin{cases} r^{L_v+1} \sum_{m=0}^{3} C_m r^{2m} & \text{for} \quad r \leqslant r_c \\ \phi(r) & \text{for} \quad r > r_c \end{cases}$$

  与 Troullier-Martin NC 方案类似，逆向求解本征方程得到有效赝势

- Bessel 方案
  直接构造有效赝势 $V_{\text{eff}}^{PS}(r) = \alpha \cdot \dfrac{\sin(q \cdot r)}{r}$

赝分波函数与投影子函数构造

- Blöchl 方法
  引入截断函数 $k(r)$

$$k(r) = \begin{cases} \left[\dfrac{\sin(\pi r/r_c)}{(\pi r/r_c)}\right]^2 & \text{for} \quad r < r_c \\ 0 & \text{for} \quad r \geqslant r_c \end{cases}$$

构造有效 (局域) 赝势 $\tilde{v}_{\mathrm{at}}$，得到广义本征值方程

$$(\tilde{H}(\vec{r}) - \epsilon_i)|\tilde{\phi}_i^0(\vec{r})\rangle = C_i k(r)|\tilde{\phi}_i^0(\vec{r})\rangle$$

迭代求解得到初始赝分波 $\phi_i^0(\vec{r})$

生成初始投影子函数 $|\tilde{p}_i^0(\vec{r})\rangle = \dfrac{k(r)|\tilde{\phi}_i^0(\vec{r})\rangle}{\langle\phi_i^0|k|\phi_i^0\rangle}$

并且初始投影函数与初始赝分波满足归一化条件(不要求正交)

$$\langle\psi_i^0|\tilde{p}_i^0\rangle = 1$$

意味着广义本征值方程可以表示为

$$\left(\tilde{H}(\mathbf{r}) - \varepsilon_i\right)|\tilde{\phi}_i^0(\mathbf{r})\rangle = |\tilde{p}_i^0(\mathbf{r})\rangle\langle\psi_i^0|\tilde{H}(\mathbf{r}) - \varepsilon_i|\tilde{\psi}_i^0\rangle$$

采用 Gram-Schmidt 正交化确定最终的赝分波和投影函数

赝分波函数与投影子函数构造

- Vanderbilt 方法
  采用多项式构造赝分波函数，要求满足

$$\tilde{\phi}_i(r) = \begin{cases} r^{l+1}\sum\limits_{m=0}^{4} C_m r^{2m} & \text{for} \quad r < r_c \\ \phi_l(r) & \text{for} \quad r \geqslant r_c \end{cases}$$

构造赝分波的辅助函数

$$\chi_l(r) = \left(\epsilon_l + \frac{\hbar^2}{2m}(\frac{\mathrm{d}^2}{\mathrm{d}r^2}) - \frac{l(l+1)}{r^2} - V_{\mathrm{eff}}^{PS}(r)\right)\tilde{\phi}_l(r)$$

和变换矩阵 $\mathbf{B}$(其矩阵元 $B_{ij} = \int_0^{r_c}\mathrm{d}r\tilde{\phi}_i(r)\chi_j(r)$)
由此得到投影子函数 $\tilde{p}_i(\vec{r}) = \sum\limits_j \chi_j(r)(\mathbf{B}^{-1})_{ji}$

AtomPAW 程序的赝势构造

赝分波函数与投影子函数构造

- RRKJ 方法
  采用球 Bessel 函数构造赝分波函数，要求满足

$$\tilde{\phi}_i = \begin{cases} r \cdot \left(\alpha_1^l \cdot j_l(q_1^l r) + \alpha_2^l \cdot j_l(q_2^l r) \right) & \text{for} \quad r < r_c \\ \phi_l(r) & \text{for} \quad r \geqslant r_c \end{cases}$$

投影子函数的构造与 Vanderbilt 方法类似

- 赝分波电荷密度的计算

$$\tilde{n}(r) = \sum_{n,l} c_{n,l} \frac{|\tilde{\phi}_{n,l}(r)|^2}{4\pi r^2}$$

- 赝芯波电荷密度的计算

$$4\pi r^2 \tilde{n}_{core}(r) = \begin{cases} r^2(U_0 + U_2 r^2 + U_4 r^4) & \text{for} \quad r \leqslant r_c \\ 4\pi r^2 n_{core}(r) & \text{for} \quad r > r_c \end{cases}$$

- 补充电荷的构造

$$\hat{n}(r) = \left(-Z + \int \mathrm{d}^3 r [n_{core}(r) + n(r) - \tilde{n}_{core}(r) - \tilde{n}(r)] \right) g_{00}(r)$$

形状函数 g_{LM} 的定义为

$$g_{LM}(r) = N_L r^L k(r) Y_{LM}(\hat{r})$$

根据 $k(r)$ 的不同可以取 sinc、Gaussian 或 Bessel 型等几种

- 局域势函数 (可移植的“赝势”)

$$\tilde{v}_{loc}(r) = V_{\mathrm{eff}}^{PS}(r) - e^2 \int \mathrm{d}^3 r' \frac{\tilde{n}_{core}(r') + \tilde{n}(r') + \hat{n}(r')}{|r - r'|} - \mu_{XC}[\tilde{n}_{core}(r) + \tilde{n}(r)]$$

AtomPAW 程序的赝势构造

- 相关矩阵元的计算
  AtomPAW 完成了与原子分波、赝分波有关的矩阵元 D^{α}_{ij}、O^{α}_{ij} 的计算
  此外还计算了

$$W^{\alpha}_{ij} = \sum_{nl} c_{n\vec{k}} \langle \tilde{\Psi}_{n\vec{k}} | \tilde{p}^{\alpha}_i \rangle \langle \tilde{p}^{\alpha}_j | \tilde{\Psi}_{n\vec{k}} \rangle$$

实际计算中，$\tilde{\Psi}_{n\vec{k}}$ 用平面波展开，于是

$$\langle \tilde{p}^{\alpha}_i | \tilde{\Psi}_{n\vec{k}} \rangle = \sqrt{\frac{1}{V}} \sum_{\vec{G}} \left(4\pi \mathrm{i}^{l}_{i} Y^{*}_{l_i m_i} (\widehat{\vec{k}+\vec{G}}) \mathrm{e}^{\mathrm{i}(\vec{k}+\vec{G})\cdot\vec{R}_{\alpha}} \right) \tilde{\tilde{p}}_{n_i l_i}(|\vec{k}+\vec{G}|) A_{n\vec{k}}(\vec{G})$$

这里

$$\tilde{\tilde{p}}_{n_i l_i}(\vec{q}) = \int_0^{r^{\alpha}_c} \mathrm{d}r r \tilde{p}_{n_i l_i}(r) j_{l_i}(\vec{q}\cdot\vec{r})$$

```
 PAW_PBE Si 05Jan2001
 4.00000000000000000
 parameters from PSCTR are:
   VRHFIN =Si: s2p2
   LEXCH  = PE
   EATOM  =   103.0669 eV,    7.5752 Ry

   TITEL  = PAW_PBE Si 05Jan2001
   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  =    2.480; RWIGS  =    1.312    wigner-seitz radius (au A)
   ENMAX  =  245.345; ENMIN  =  184.009 eV
   ICORE  =        2    local potential
   LCOR   =        T    correct aug charges
   LPAW   =        T    paw PP
   EAUG   =  322.069
   DEXC   =    -.007
   RMAX   =    2.944    core radius for proj-oper
   RAUG   =    1.300    factor for augmentation sphere
   RDEP   =    1.993    radius for radial grids
   QCUT   =   -4.246; QGAM   =    8.493    optimization parameters

   Description
     l     E        TYP  RCUT    TYP  RCUT
     0    .000      23  1.900
     0    .000      23  1.900
     1    .000      23  1.900
     1    .000      23  1.900
     2    .000       7  1.900
   Error from kinetic energy argument (eV)
   NDATA  =      100
   STEP   =   20.000   1.050
  10.1      9.04      8.56      7.65      7.23      6.44      5.73      5.40
  4.79      4.25      4.00      3.54      3.13      2.77      2.45      2.16
  1.91      1.69      1.50      1.24      1.10      .975      .812      .718
  .636      .529      .440      .388      .322      .266      .219      .180
  .148      .121      .986E-01  .804E-01  .614E-01  .504E-01  .392E-01  .328E-01
  .265E-01  .220E-01  .189E-01  .166E-01  .149E-01  .135E-01  .123E-01  .109E-01
  .977E-02  .840E-02  .707E-02  .605E-02  .488E-02  .387E-02  .290E-02  .229E-02
  .185E-02  .152E-02  .134E-02  .125E-02  .121E-02  .117E-02  .112E-02  .102E-02
  .915E-03  .776E-03  .640E-03  .524E-03  .425E-03  .369E-03  .331E-03  .310E-03
  .294E-03  .273E-03  .242E-03  .210E-03  .175E-03  .146E-03  .124E-03  .113E-03
  .105E-03  .973E-04  .879E-04  .755E-04  .633E-04  .539E-04  .478E-04  .438E-04
  .404E-04  .362E-04  .308E-04  .264E-04  .229E-04  .209E-04  .192E-04  .170E-04
  .145E-04  .126E-04  .112E-04  .103E-04
END of PSCTR-controll parameters
```

VASP 的 POTCAR

```
 local part
 98.2657514061040160
   .84157696E+01   .84210616E+01   .84276868E+01   .84387430E+01   .84542501E+01
   .84742336E+01   .84987229E+01   .85277486E+01   .85613410E+01   .85995276E+01
   .86423322E+01   .86897735E+01   .87418643E+01   .87986117E+01   .88600162E+01
   .89260725E+01   .89967686E+01   .90720854E+01   .91519966E+01   .92364669E+01
   .93254512E+01   .94188926E+01   .95167214E+01   .96188530E+01   .97251866E+01
   .98356042E+01   .99499691E+01   .10068126E+02   .10189900E+02   .10315095E+02
   .10443498E+02   .10574872E+02   .10708964E+02   .10845497E+02   .10984178E+02
   .11124691E+02   .11266702E+02   .11409858E+02   .11553785E+02   .11698096E+02
   .11842382E+02   .11986223E+02   .12129182E+02   .12270810E+02   .12410650E+02
   .12548232E+02   .12683081E+02   .12814718E+02   .12942658E+02   .13066416E+02
   .13185509E+02   .13299456E+02   .13407780E+02   .13510014E+02   .13605699E+02
   .13694388E+02   .13775652E+02   .13849074E+02   .13914259E+02   .13970835E+02
   .14018449E+02   .14056778E+02   .14085523E+02   .14104415E+02   .14113216E+02
   .14111719E+02   .14099752E+02   .14077176E+02   .14043889E+02   .13999825E+02
   .13944955E+02   .13879288E+02   .13802872E+02   .13715793E+02   .13618173E+02
   .13510175E+02   .13391996E+02   .13263872E+02   .13126073E+02   .12978903E+02
   .12822702E+02   .12657838E+02   .12484712E+02   .12303753E+02   .12115415E+02
   .11920177E+02   .11718543E+02   .11511033E+02   .11298186E+02   .11080557E+02
   .10858712E+02   .10633228E+02   .10404688E+02   .10173679E+02   .99407918E+01
   .97066146E+01   .94717325E+01   .92367246E+01   .90021609E+01   .87686001E+01
   .85365874E+01   .83066514E+01   .80793026E+01   .78550308E+01   .76343035E+01
   .74175636E+01   .72052280E+01   .69976861E+01   .67952984E+01   .65983952E+01
   .64072758E+01   .62222076E+01   .60434252E+01   .58711303E+01   .57054911E+01
   .55466426E+01   .53946862E+01   .52496902E+01   .51116906E+01   .49806911E+01
   .48566645E+01   .47395534E+01   .46292712E+01   .45257038E+01   .44287105E+01
   .43381258E+01   .42537607E+01   .41754049E+01   .41028282E+01   .40357822E+01
   .39740031E+01   .39172124E+01   .38651203E+01   .38174267E+01   .37738238E+01
   .37339979E+01   .36976315E+01   .36644056E+01   .36340010E+01   .36061008E+01
   .35803917E+01   .35565663E+01   .35343243E+01   .35133745E+01   .34934357E+01
   .34742388E+01   .34555274E+01   .34370596E+01   .34186083E+01   .33999627E+01
   .33809285E+01   .33613290E+01   .33410052E+01   .33198164E+01   .32976401E+01
   .32743723E+01   .32499276E+01   .32242387E+01   .31972561E+01   .31689481E+01
   .31393000E+01   .31083133E+01   .30760055E+01   .30424087E+01   .30075693E+01
   .29715463E+01   .29344112E+01   .28962459E+01   .28571426E+01   .28172018E+01
   .27765317E+01   .27352466E+01   .26934662E+01   .26513138E+01   .26089155E+01
   .25663991E+01   .25238927E+01   .24815236E+01   .24394173E+01   .23976966E+01
   .23564804E+01   .23158831E+01   .22760134E+01   .22369739E+01   .21988600E+01
   .21617599E+01   .21257533E+01   .20909116E+01   .20572974E+01   .20249638E+01
   .19939548E+01   .19643045E+01   .19360379E+01   .19091701E+01   .18837069E+01
   .18596450E+01   .18369720E+01   .18156670E+01   .17957010E+01   .17770368E+01
   .17596305E+01   .17434311E+01   .17283816E+01   .17144193E+01   .17014768E+01
   .16894823E+01   .16783607E+01   .16680338E+01   .16584212E+01   .16494415E+01
   .16410120E+01   .16330504E+01   .16254746E+01   .16182040E+01   .16111597E+01
   .16042653E+01   .15974473E+01   .15906355E+01   .15837638E+01   .15767703E+01
   .15695978E+01   .15621941E+01   .15545123E+01   .15465111E+01   .15381544E+01
   .15294125E+01   .15202610E+01   .15106817E+01   .15006619E+01   .14901947E+01
   .14792788E+01   .14679182E+01   .14561221E+01   .14439046E+01   .14312844E+01
   .14182846E+01   .14049321E+01   .13912574E+01   .13772942E+01   .13630791E+01
   .13486509E+01   .13340503E+01   .13193195E+01   .13045019E+01   .12896412E+01
   .12747815E+01   .12599666E+01   .12452397E+01   .12306428E+01   .12162167E+01
   .12020006E+01   .11880314E+01   .11743437E+01   .11609697E+01   .11479386E+01
   .11352766E+01   .11230067E+01   .11111486E+01   .10997186E+01   .10887293E+01
   .10781902E+01   .10681067E+01   .10584813E+01   .10493127E+01   .10405964E+01
   .10323246E+01   .10244865E+01   .10170685E+01   .10100542E+01   .10034245E+01
   .99715846E+00   .99123280E+00   .98562260E+00   .98030145E+00   .97524173E+00
   .97041488E+00   .96579171E+00   .96134265E+00   .95703806E+00   .95284844E+00
   .94874473E+00   .94469858E+00   .94068254E+00   .93667031E+00   .93263696E+00
   .92855909E+00   .92441506E+00   .92018509E+00   .91585142E+00   .91139842E+00
   .90681263E+00   .90208291E+00   .89720039E+00   .89215854E+00   .88695315E+00
   .88158229E+00   .87604630E+00   .87034770E+00   .86449110E+00   .85848313E+00
   .85233229E+00   .84604884E+00   .83964465E+00   .83313300E+00   .82652847E+00
   .81984671E+00   .81310428E+00   .80631845E+00   .79950703E+00   .79268813E+00
   .77677943E-01   .77559095E-01   .77435971E-01   .77308267E-01   .77175728E-01
...............................................................................
...............................................................................

   .77038154E-01   .76895403E-01   .76747386E-01   .76594073E-01   .76435492E-01
   .76271726E-01   .76102913E-01   .75929245E-01   .75750968E-01   .75568374E-01
 gradient corrections used for XC
 5
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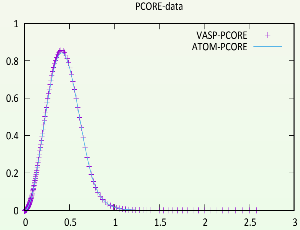

VASP 的 POTCAR


```
core charge-density (partial)
  .13681950E+01  .13676960E+01  .13662001E+01  .13637105E+01  .13602325E+01
  .13557734E+01  .13503429E+01  .13439524E+01  .13366153E+01  .13283473E+01
  .13191655E+01  .13090892E+01  .12981393E+01  .12863384E+01  .12737107E+01
  .12602820E+01  .12460794E+01  .12311314E+01  .12154677E+01  .11991194E+01
  .11821181E+01  .11644970E+01  .11462895E+01  .11275301E+01  .11082538E+01
  .10884962E+01  .10682931E+01  .10476808E+01  .10266957E+01  .10053741E+01
  .98375267E+00  .96186759E+00  .93975503E+00  .91745077E+00  .89499021E+00
  .87240826E+00  .84973926E+00  .82701690E+00  .80427415E+00  .78154320E+00
  .75885536E+00  .73624104E+00  .71372967E+00  .69134969E+00  .66912843E+00
  .64709213E+00  .62526592E+00  .60367371E+00  .58233824E+00  .56128104E+00
  .54052238E+00  .52008130E+00  .49997559E+00  .48022178E+00  .46083513E+00
  .44182968E+00  .42321820E+00  .40501225E+00  .38722216E+00  .36985707E+00
  .35292495E+00  .33643262E+00  .32038578E+00  .30478902E+00  .28964588E+00
  .27495886E+00  .26072949E+00  .24695832E+00  .23364498E+00  .22078822E+00
  .20838596E+00  .19643530E+00  .18493258E+00  .17387344E+00  .16325283E+00
  .15306507E+00  .14330386E+00  .13396240E+00  .12503332E+00  .11650883E+00
  .10838067E+00  .10064023E+00  .93278522E-01  .86286250E-01  .79653846E-01
  .73371505E-01  .67429216E-01  .61816797E-01  .56523934E-01  .51540202E-01
  .46855108E-01  .42458109E-01  .38338647E-01  .34486174E-01  .30890174E-01
  .27540191E-01  .24425850E-01  .21536879E-01  .18863125E-01  .16394577E-01
  .14121382E-01  .12033860E-01  .10122516E-01  .83780589E-02  .67914092E-02
  .53537108E-02  .40563408E-02  .28909177E-02  .18493086E-02  .92363545E-03
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 -.26037134E-02 -.29161762E-02 -.31661368E-02 -.33590603E-02 -.35001462E-02
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 -.35166058E-02 -.34188439E-02 -.33017396E-02 -.31682957E-02 -.30213004E-02
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 -.19856525E-02 -.18053531E-02 -.16269545E-02 -.14516446E-02 -.12804716E-02
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 -.38329201E-03 -.26025656E-03 -.14560117E-03 -.39444206E-04  .58165516E-04
  .14724263E-03  .22785937E-03  .30013989E-03  .36425487E-03  .42041630E-03
  .46887251E-03  .50990347E-03  .54381628E-03  .57094091E-03  .59162620E-03
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  .60152031E-03  .58774722E-03  .57059965E-03  .55045362E-03  .52767640E-03
  .50262485E-03  .47564400E-03  .44706580E-03  .41720805E-03  .38637350E-03
  .35484906E-03  .32290522E-03  .29079555E-03  .25875641E-03  .22700669E-03
  .19574775E-03  .16516340E-03  .13542004E-03  .10666685E-03  .79036088E-04
  .52643451E-04  .27588517E-04  .39552464E-05 -.18187465E-04 -.38785178E-04
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  .44531079E-04  .47412645E-04  .49828605E-04  .51786930E-04  .53298094E-04
  .54374884E-04  .55032195E-04  .55286832E-04  .55157309E-04  .54663646E-04
  .53827166E-04  .52670302E-04  .51216402E-04  .49489534E-04  .47514310E-04
  .45315700E-04  .42918863E-04  .40348986E-04  .37631124E-04  .34790051E-04
  .31850126E-04  .28835162E-04  .25768303E-04  .22671916E-04  .19567494E-04
  .16475560E-04  .13415592E-04  .10405948E-04  .74638126E-05  .46051404E-05
  .18446197E-05 -.80436009E-06 -.33297302E-05 -.57207550E-05 -.79680369E-05
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  .97604944E-05  .95548661E-05  .92952495E-05  .89852710E-05  .86287366E-05
  .82296019E-05  .77919423E-05  .73199237E-05  .68177739E-05  .62897539E-05
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 -.13688530E-05 -.10675792E-05 -.76892250E-06 -.47467171E-06 -.18653188E-06
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```

VASP 的 POTCAR

```
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  .36801845E+01  .35492225E+01  .34014950E+01  .32399100E+01  .30674335E+01
  .28869885E+01  .27013712E+01  .25131849E+01  .23247937E+01  .21382919E+01
  .19554911E+01  .17779180E+01  .16068237E+01  .14431992E+01  .12877965E+01
  .11411517E+01  .10036103E+01  .87535141E+00  .75641220E+00  .64671001E+00
  .54606321E+00  .45420994E+00  .37082490E+00  .29553413E+00  .22792793E+00
  .16757210E+00  .11401744E+00  .66807913E-01  .25487409E-01 -.10394612E-01
 -.41278562E-01 -.67591071E-01 -.89742138E-01 -.10812299E+00 -.12310456E+00
 -.13503646E+00 -.14424640E+00 -.15104001E+00 -.15570097E+00 -.15849133E+00
 -.15965211E+00 -.15940402E+00 -.15794831E+00 -.15546772E+00 -.15212749E+00
 -.14807638E+00 -.14344771E+00 -.13836047E+00 -.13292033E+00 -.12722065E+00
 -.12134348E+00 -.11536052E+00 -.10933401E+00 -.10331756E+00 -.97357004E-01
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  .39911853E-03  .36326031E-03  .32650377E-03  .28945387E-03  .25263036E-03
  .21647525E-03  .18135985E-03  .14759141E-03  .11541928E-03  .85040816E-04
  .56606764E-04  .30226352E-04  .59719919E-05 -.16116354E-04 -.36027141E-04
 -.53773520E-04 -.69389928E-04 -.82928949E-04 -.94458459E-04 -.10405902E-03
 -.11182151E-03 -.11784499E-03 -.12223478E-03 -.12510073E-03 -.12655567E-03
 -.12671407E-03 -.12569076E-03 -.12359997E-03 -.12055430E-03 -.11666399E-03
 -.11203621E-03 -.10677448E-03 -.10097820E-03 -.94742231E-04 -.88156609E-04
 -.81306283E-04 -.74270942E-04 -.67124899E-04 -.59937023E-04 -.52770714E-04
 -.45683928E-04 -.38729233E-04 -.31953896E-04 -.25400000E-04 -.19104585E-04
 -.13099806E-04 -.74131135E-05 -.20674438E-05  .29185776E-05  .75304221E-05
  .11757438E-04  .15592625E-04  .19032404E-04  .22076388E-04  .24727147E-04
  .26989979E-04  .28872677E-04  .30385308E-04  .31539981E-04  .32350635E-04
  .32832821E-04  .33003493E-04  .32880805E-04  .32483918E-04  .31832808E-04
  .30948085E-04  .29850818E-04  .28562372E-04  .27104248E-04  .25497933E-04
  .23764761E-04  .21925781E-04  .20001631E-04  .18012428E-04  .15977661E-04
  .13916095E-04  .11845684E-04  .97834913E-05  .77456253E-05  .57471751E-05
  .38021614E-05  .19234941E-05  .12293798E-06 -.15889121E-05 -.32026485E-05
 -.47100596E-05 -.61041317E-05 -.73790420E-05 -.85301460E-05 -.95539569E-05
 -.10448119E-04 -.11211374E-04 -.11843524E-04 -.12345387E-04 -.12718747E-04
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 -.12467816E-04 -.12060693E-04 -.11567014E-04 -.10994484E-04 -.10351114E-04
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 -.54732369E-05 -.45696518E-05 -.36621723E-05 -.27585615E-05 -.18662606E-05
 -.99234299E-06 -.14347216E-06  .67413606E-06  .14547465E-05  .21931331E-05
  .28846026E-05  .35250133E-05  .41107897E-05  .46389311E-05  .51070171E-05
  .55132071E-05  .58562363E-05  .61354066E-05  .63505743E-05  .65021328E-05
  .65909923E-05  .66185560E-05  .65866927E-05  .64977074E-05  .63543081E-05
  .61595714E-05  .59169057E-05  .56300130E-05  .53028493E-05  .49395841E-05
  .45445596E-05  .41222492E-05  .36772171E-05  .32140765E-05  .27374510E-05
  .22519347E-05  .17620554E-05  .12722380E-05  .78677129E-06  .30977508E-06
 -.15482897E-06 -.60334483E-06 -.10323267E-05 -.14386008E-05 -.18192846E-05
 -.21718029E-05 -.24939006E-05 -.27836530E-05 -.30394730E-05 -.32601147E-05
 -.34446746E-05 -.35925898E-05 -.37036332E-05 -.37779061E-05 -.38158282E-05
 -.38181253E-05 -.37858143E-05 -.37201867E-05 -.36227899E-05 -.34954069E-05
 -.33400340E-05 -.31588583E-05 -.29542334E-05 -.27286543E-05 -.24847319E-05
 -.22251674E-05 -.19527264E-05 -.16702126E-05 -.13804427E-05 -.10862214E-05
 -.79031713E-06 -.49543860E-06 -.20421280E-06  .80835994E-07  .35730573E-06
  .62293455E-06  .87561703E-06  .11134188E-05  .13345890E-05  .15375714E-05
  .17210128E-05  .18837700E-05  .20249147E-05  .21437361E-05  .22397418E-05
  .23126566E-05  .23624198E-05  .23891799E-05  .23932885E-05  .23752919E-05
  .23359216E-05  .22760829E-05  .21968428E-05  .20994165E-05  .19851530E-05
  .18555195E-05  .17120855E-05  .15565066E-05  .13905072E-05  .12158635E-05
  .10343865E-05  .84790465E-06  .65824737E-06  .46722828E-06  .27662940E-06
  .88185931E-07 -.96428306E-07 -.27561447E-06 -.44786132E-06 -.61175681E-06
 -.76599844E-06 -.90940250E-06 -.10409120E-05 -.11596031E-05 -.12646906E-05
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 -.14419091E-05 -.13742618E-05 -.12953968E-05 -.12062995E-05 -.11080263E-05
 -.10016944E-05 -.88846949E-06 -.76955446E-06 -.64617751E-06 -.51958041E-06
 -.39100686E-06 -.26169110E-06 -.13284687E-06 -.56567587E-08  .11873791E-06
  .23924662E-06  .35483853E-06  .46455060E-06  .56749495E-06  .66286537E-06
  .74994293E-06  .82810073E-06  .89680762E-06  .95563110E-06  .10042391E-05
  .10424010E-05  .10699876E-05  .10869699E-05  .10934176E-05  .10894963E-05
  .10754638E-05  .10516660E-05  .10185318E-05  .97656733E-06  .92634993E-06
  .86852113E-06  .80377954E-06  .73287323E-06  .65659178E-06  .57575821E-06
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VASP 的 POTCAR

```
19.8421228800786942 T
Non local Part
0 2 1.55770284366884382
8.48191151414740752 -0.636078516188222226E-01 -0.636078516188222226E-01 0.376965742998787998E-02
Reciprocal Space Part
  .87079657E+01  .86905268E+01  .86383852E+01  .85520639E+01  .84324261E+01
  .82806628E+01  .80982759E+01  .78870568E+01  .76490608E+01  .73865785E+01
  .71021037E+01  .67982989E+01  .64779593E+01  .61439752E+01  .57992933E+01
  .54468791E+01  .50896789E+01  .47305835E+01  .43723936E+01  .40177873E+01
  .36692907E+01  .33292513E+01  .29998152E+01  .26829081E+01  .23802200E+01
  .20931942E+01  .18230205E+01  .15706325E+01  .13367087E+01  .11216776E+01
  .92572621E+00  .74881221E+00  .59067848E+00  .45087066E+00  .32875652E+00
  .22354716E+00  .13431939E+00  .60038835E-01 -.41655140E-03 -.48233192E-01
 -.84639053E-01 -.11088174E+00 -.12820783E+00 -.13784377E+00 -.14097860E+00
 -.13874855E+00 -.13222400E+00 -.12239850E+00 -.11018019E+00 -.96385516E-01
 -.81735140E-01 -.66852083E-01 -.52261834E-01 -.38394355E-01 -.25587745E-01
 -.14093369E-01 -.40822094E-02  .43477954E-02  .11163663E-01  .16388781E-01
  .20094049E-01  .22388976E-01  .23412932E-01  .23326746E-01  .22304805E-01
  .20527794E-01  .18176188E-01  .15424571E-01  .12436845E-01  .93623490E-02
  .63329000E-02  .34607215E-02  .83723118E-03 -.14673812E-02 -.34038583E-02
 -.49429505E-02 -.60739569E-02 -.68028370E-02 -.71499932E-02 -.71478312E-02
 -.68381952E-02 -.62697733E-02 -.54955578E-02 -.45704368E-02 -.35489799E-02
 -.24834728E-02 -.14222372E-02 -.40826592E-03  .52181480E-03  .13384515E-02
  .20195476E-02  .25505425E-02  .29242131E-02  .31402290E-02  .32045017E-02
  .31283679E-02  .29276511E-02  .26216452E-02  .22320639E-02  .17819939E-02
Real Space Part
  .10679849E+02  .10674516E+02  .10658521E+02  .10631882E+02  .10594629E+02
  .10546798E+02  .10488435E+02  .10419590E+02  .10340316E+02  .10250666E+02
  .10150691E+02  .10040442E+02  .99199643E+01  .97892993E+01  .96484877E+01
  .94975699E+01  .93365905E+01  .91656025E+01  .89846735E+01  .87938923E+01
  .85933769E+01  .83832826E+01  .81638104E+01  .79352160E+01  .76978177E+01
  .74520045E+01  .71982421E+01  .69370789E+01  .66691491E+01  .63951751E+01
  .61159665E+01  .58324186E+01  .55455066E+01  .52562794E+01  .49658496E+01
  .46753825E+01  .43860825E+01  .40991787E+01  .38159080E+01  .35374987E+01
  .32651527E+01  .30000279E+01  .27432213E+01  .24957525E+01  .22585487E+01
  .20324314E+01  .18181051E+01  .16161478E+01  .14270049E+01  .12509847E+01
  .10882570E+01  .93885502E+00  .80267855E+00  .67950082E+00  .56897697E+00
  .47065459E+00  .38398603E+00  .30834185E+00  .24302540E+00  .18728774E+00
  .14034296E+00  .10138309E+00  .69592617E-01  .44162070E-01  .24300516E-01
  .92466753E-02 -.17214853E-02 -.92788061E-02 -.14046714E-01 -.16588732E-01
 -.17407693E-01 -.16944568E-01 -.15578795E-01 -.13629958E-01 -.11360623E-01
 -.89801560E-02 -.66492956E-02 -.44852808E-02 -.25673264E-02 -.94224811E-03
  .36993817E-03  .13706046E-02  .20774200E-02  .25196886E-02  .27342003E-02
  .27616467E-02  .26436316E-02  .24202815E-02  .21284366E-02  .18003892E-02
  .14631174E-02  .11379537E-02  .84061912E-03  .58155029E-03  .36644718E-03
  .19697068E-03  .71525435E-04 -.13929925E-04 -.65094077E-04 -.88595362E-04
Reciprocal Space Part
 -.33459269E+02 -.32885812E+02 -.31175324E+02 -.28357261E+02 -.24480084E+02
 -.19610327E+02 -.13831310E+02 -.72415472E+01  .47142272E-01  .79117577E+01
  .16220445E+02  .24834975E+02  .33613317E+02  .42412261E+02  .51090027E+02
  .59508819E+02  .67537255E+02  .75052646E+02  .81943063E+02  .88109160E+02
  .93465720E+02  .97942900E+02  .10148714E+03  .10406175E+03  .10564715E+03
  .10624077E+03  .10585660E+03  .10452449E+03  .10228909E+03  .99208571E+02
  .95353099E+02  .90803154E+02  .85647663E+02  .79982052E+02  .73906232E+02
  .67522572E+02  .60933898E+02  .54241560E+02  .47543611E+02  .40933123E+02
  .34496680E+02  .28313063E+02  .22452162E+02  .16974111E+02  .11928669E+02
  .73548473E+01  .32807727E+01 -.27621319E+00 -.33092347E+01 -.58213610E+01
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 -.72003946E+01 -.60361114E+01 -.48487123E+01 -.36743572E+01 -.25447982E+01
 -.14870336E+01 -.52310141E+00  .32999049E+00  .10602053E+01  .16603003E+01
  .21275436E+01  .24633402E+01  .26727834E+01  .27641476E+01  .27483410E+01
  .26383351E+01  .24485880E+01  .21944773E+01  .18917574E+01  .15560536E+01
  .12024051E+01  .84486462E+00  .49616263E+00  .16743966E+00 -.13195032E+00
 -.39456569E+00 -.61493394E+00 -.78954326E+00 -.91677435E+00 -.99677914E+00
 -.10313144E+01 -.10235387E+01 -.97778206E+00 -.89929746E+00 -.79400304E+00
 -.66822444E+00 -.52844495E+00 -.38107084E+00 -.23221848E+00 -.87528095E-01
Real Space Part
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  .47404142E+03  .47502541E+03  .47573899E+03  .47598368E+03  .47554935E+03
  .47422109E+03  .47178640E+03  .46804221E+03  .46280172E+03  .45590085E+03
  .44720395E+03  .43660875E+03  .42405037E+03  .40950423E+03  .39298784E+03
  .37456135E+03  .35432699E+03  .33242725E+03  .30904200E+03  .28438464E+03
  .25869730E+03  .23224536E+03  .20531141E+03  .17818879E+03  .15117498E+03
  .12456500E+03  .98644898E+02  .73685748E+02  .49938027E+02  .27626718E+02
  .69471588E+01 -.11938243E+02 -.28902388E+02 -.43854906E+02 -.56742633E+02
 -.67549163E+02 -.76293525E+02 -.83028062E+02 -.87835614E+02 -.90826098E+02
 -.92132623E+02 -.91907271E+02 -.90316654E+02 -.87537414E+02 -.83751758E+02
 -.79143172E+02 -.73892400E+02 -.68173791E+02 -.62152082E+02 -.55979677E+02
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VASP 的 POTCAR


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Non local Part
1 2 1.55770284366884382
2.65859659160385764 -0.504801881867953453E-01 -0.504801881867953453E-01 0.892956271679604986E-02
Reciprocal Space Part
  .00000000E+00   .55360975E+00   .11020032E+01   .16400357E+01   .21627048E+01
  .26652186E+01   .31430596E+01   .35920450E+01   .40083810E+01   .43887098E+01
  .47301505E+01   .50303314E+01   .52874138E+01   .55001078E+01   .56676786E+01
  .57899444E+01   .58672657E+01   .59005262E+01   .58911063E+01   .58408488E+01
  .57520191E+01   .56272596E+01   .54695387E+01   .52820975E+01   .50683934E+01
  .48320418E+01   .45767578E+01   .43062991E+01   .40244089E+01   .37347632E+01
  .34409202E+01   .31462743E+01   .28540152E+01   .25670915E+01   .22881811E+01
  .20196669E+01   .17636193E+01   .15217840E+01   .12955770E+01   .10860853E+01
  .89407229E+00   .71998985E+00   .56399389E+00   .42596477E+00   .30553088E+00
  .20209532E+00   .11486458E+00   .42878783E-01  -.14957234E-01  -.59842780E-01
 -.93050595E-01  -.11589722E+00  -.12971495E+00  -.13582584E+00  -.13551809E+00
 -.13002523E+00  -.12050824E+00  -.10804072E+00  -.93597327E-01  -.78045331E-01
 -.62139262E-01  -.46518532E-01  -.31707803E-01  -.18119864E-01  -.60607310E-02
  .42633380E-02   .12737265E-01   .19327344E-01   .24070560E-01   .27063374E-01
  .28450306E-01   .28412605E-01   .27157313E-01   .24906934E-01   .21889935E-01
  .18332245E-01   .14449871E-01   .10442718E-01   .64896733E-02   .27449375E-02
 -.66440255E-03  -.36396321E-02  -.61105795E-02  -.80348118E-02  -.93959825E-02
 -.10201473E-01  -.10479476E-01  -.10275671E-01  -.96496464E-02  -.86712031E-02
 -.74166865E-02  -.59654538E-02  -.43965915E-02  -.27859668E-02  -.12036827E-02
  .28801366E-03   .16363396E-02   .27990903E-02   .37452630E-02   .44552150E-02
Real Space Part
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  .31948350E+01   .38202017E+01   .44373750E+01   .50443910E+01   .56390587E+01
  .62189597E+01   .67814592E+01   .73237268E+01   .78427678E+01   .83354645E+01
  .87986250E+01   .92290406E+01   .96235469E+01   .99790905E+01   .10292796E+02
  .10562036E+02   .10784491E+02   .10958218E+02   .11081699E+02   .11153897E+02
  .11174283E+02   .11142876E+02   .11060254E+02   .10927558E+02   .10746490E+02
  .10519290E+02   .10248709E+02   .99379673E+01   .95907014E+01   .92109083E+01
  .88028781E+01   .83711229E+01   .79203026E+01   .74551481E+01   .69803858E+01
  .65006629E+01   .60204776E+01   .55441132E+01   .50755794E+01   .46185613E+01
  .41763765E+01   .37519415E+01   .33477477E+01   .29658468E+01   .26078460E+01
  .22749116E+01   .19677819E+01   .16867871E+01   .14318761E+01   .12026495E+01
  .99839626E+00   .81813432E+00   .66065330E+00   .52455802E+00   .40831211E+00
  .31028032E+00   .22876897E+00   .16206345E+00   .10846228E+00   .66307278E-01
  .34009364E-01   .10069850E-01  -.69027801E-02  -.18180606E-01  -.24908286E-01
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 -.17472311E-01  -.13679034E-01  -.10073742E-01  -.68123372E-02  -.39901212E-02
 -.16530358E-02   .19178102E-03   .15663369E-02   .25131785E-02   .30879320E-02
  .33530317E-02   .33726336E-02   .32086679E-02   .29179506E-02   .25502513E-02
  .21471944E-02   .17418610E-02   .13589554E-02   .10154019E-02   .72124547E-03
  .48074009E-03   .29352474E-03   .15580136E-03   .61447592E-04   .30138377E-05
Reciprocal Space Part
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 -.11720983E+02  -.13142152E+02  -.14093748E+02  -.14524661E+02  -.14395175E+02
 -.13677819E+02  -.12357950E+02  -.10434056E+02  -.79177661E+01  -.48335806E+01
 -.12183197E+01   .28796906E+01   .74016747E+01   .12279682E+02   .17438045E+02
  .22794994E+02   .28264383E+02   .33757491E+02   .39184855E+02   .44458102E+02
  .49491724E+02   .54204777E+02   .58522445E+02   .62377462E+02   .65711339E+02
  .68475389E+02   .70631527E+02   .72152827E+02   .73023834E+02   .73240630E+02
  .72810652E+02   .71752282E+02   .70094218E+02   .67874635E+02   .65140188E+02
  .61944855E+02   .58348663E+02   .54416332E+02   .50215862E+02   .45817101E+02
  .41290320E+02   .36704841E+02   .32127729E+02   .27622587E+02   .23248472E+02
  .19058953E+02   .15101330E+02   .11416015E+02   .80360965E+01   .49870782E+01
  .22867940E+01  -.54504994E-01  -.20339040E+01  -.36554301E+01  -.49295269E+01
 -.58724172E+01  -.65053728E+01  -.68539157E+01  -.69469702E+01  -.68159914E+01
 -.64940905E+01  -.60151778E+01  -.54131449E+01  -.47211011E+01  -.39706812E+01
 -.31914370E+01  -.24103219E+01  -.16512754E+01  -.93491359E+00  -.27832313E+00
  .30503924E+00   .80534852E+00   .12163201E+01   .15350341E+01   .17616860E+01
  .18992752E+01   .19532440E+01   .19310803E+01   .18418981E+01   .16960073E+01
  .15044873E+01   .12787746E+01   .10302757E+01   .77001425E+00   .50831954E+00
  .25456290E+00   .16945576E-01  -.19765940E+00  -.38381089E+00  -.53754978E+00
 -.65639825E+00  -.73931205E+00  -.78659086E+00  -.79975259E+00  -.78137851E+00
Real Space Part
  .00000000E+00   .32174412E+02   .64081200E+02   .95454901E+02   .12603438E+03
  .15556504E+03   .18380101E+03   .21050740E+03   .23546257E+03   .25846040E+03
  .27931254E+03   .29785062E+03   .31392841E+03   .32742382E+03   .33824076E+03
  .34631080E+03   .35159451E+03   .35408254E+03   .35379625E+03   .35078802E+03
  .34514103E+03   .33696853E+03   .32641275E+03   .31364309E+03   .29885400E+03
  .28226227E+03   .26410388E+03   .24463049E+03   .22410561E+03   .20280043E+03
  .18098955E+03   .15894661E+03   .13693992E+03   .11522816E+03   .94056367E+02
  .73652166E+02   .54222369E+02   .35950069E+02   .18992243E+02   .34779240E+01
 -.10493014E+02  -.22850445E+02  -.33553946E+02  -.42592145E+02  -.49981475E+02
 -.55764394E+02  -.60007127E+02  -.62796996E+02  -.64239417E+02  -.64454665E+02
 -.63574472E+02  -.61738574E+02  -.59091275E+02  -.55778129E+02  -.51942809E+02
 -.47724232E+02  -.43254004E+02  -.38654223E+02  -.34035686E+02  -.29496509E+02
```

VASP 的 POTCAR


```
 PAW radial sets
 323 0.989218471734281124
(5E20.12)
 augmentation charges (non sperical)
  -.118612867153E+00  -.756362247412E-03  -.532145531503E-01  -.130926919871E-02  -.756362247412E-03
  -.210856503823E-04  -.122603249007E-03   .363423839020E-05  -.532145531503E-01  -.122603249007E-03
  -.179689875812E-01  -.555432069872E-03  -.130926919871E-02   .363423839020E-05  -.555432069872E-03
   .498671741032E-04
 uccopancies in atom
   .200000000162E+01   .000000000000E+00   .000000000000E+00   .000000000000E+00   .000000000000E+00
   .000000000000E+00   .000000000000E+00   .000000000000E+00   .000000000000E+00   .000000000000E+00
   .666666667141E+00   .000000000000E+00   .000000000000E+00   .000000000000E+00   .000000000000E+00
   .000000000000E+00
```

VASP 的 POTCAR


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grid
   .353278105438E-04  .364765828105E-04  .376627102856E-04  .388874076671E-04  .401519291522E-04
   .414575697215E-04  .428056664648E-04  .441975999512E-04  .456347956421E-04  .471187253514E-04
   .486509087530E-04  .502329149365E-04  .518663640144E-04  .535529287814E-04  .552943364272E-04
   .570923703053E-04  .589488717596E-04  .608657420098E-04  .628449440985E-04  .648885049016E-04
   .669985172040E-04  .691771418426E-04  .714266099194E-04  .737492250864E-04  .761473659044E-04
   .786234882792E-04  .811801279764E-04  .838199032186E-04  .865455173661E-04  .893597616862E-04
   .922655182109E-04  .952657626888E-04  .983635676325E-04  .101562105465E-03  .104864651768E-03
   .108274588638E-03  .111795408149E-03  .115430715926E-03  .119184234844E-03  .123059808833E-03
   .127061406819E-03  .131193126789E-03  .135459199986E-03  .139863995240E-03  .144412023447E-03
   .149107942186E-03  .153956560487E-03  .158962843759E-03  .164131918874E-03  .169469079417E-03
   .174979791106E-03  .180669697392E-03  .186544625235E-03  .192610591076E-03  .198873806993E-03
   .205340687067E-03  .212017853948E-03  .218912145639E-03  .226030622496E-03  .233380574462E-03
   .240969528530E-03  .248805256452E-03  .256895782699E-03  .265249392676E-03  .273874641209E-03
   .282780361308E-03  .291975673207E-03  .301469993709E-03  .311273045829E-03  .321394868748E-03
   .331845828098E-03  .342636626573E-03  .353778314896E-03  .365282303127E-03  .377160372357E-03
   .389424686766E-03  .402087806084E-03  .415162698451E-03  .428662753701E-03  .442601797068E-03
   .456994103352E-03  .471854411533E-03  .487197939863E-03  .503040401457E-03  .519398020380E-03
   .536287548263E-03  .553726281459E-03  .571732078754E-03  .590323379658E-03  .609519223288E-03
   .629339267864E-03  .649803810846E-03  .670933809712E-03  .692750903429E-03  .715277434606E-03
   .738536472381E-03  .762551836040E-03  .787348119413E-03  .812950716063E-03  .839385845286E-03
   .866680578963E-03  .894862869287E-03  .923961577387E-03  .954006502881E-03  .985028414399E-03
   .101705908109E-02  .105013130516E-02  .108427895544E-02  .111953700213E-02  .115594155253E-02
   .119352988810E-02  .123234050257E-02  .127241314140E-02  .131378884247E-02  .135650997813E-02
   .140062029854E-02  .144616497653E-02  .149319065382E-02  .154174548883E-02  .159187920594E-02
   .164364314647E-02  .169709032120E-02  .175227546473E-02  .180925509145E-02  .186808755348E-02
   .192883310041E-02  .199155394099E-02  .205631430683E-02  .212318051821E-02  .219222105197E-02
   .226350661166E-02  .233711019991E-02  .241310719324E-02  .249157541920E-02  .257259523611E-02
   .265624961535E-02  .274262422631E-02  .283180752413E-02  .292389084032E-02  .301896847624E-02
   .311713779968E-02  .321849934462E-02  .332315691413E-02  .343121768671E-02  .354279232604E-02
   .365799509430E-02  .377694396919E-02  .389976076474E-02  .402657125610E-02  .415750530828E-02
   .429269700920E-02  .443228480697E-02  .457641165169E-02  .472522514185E-02  .487887767547E-02
   .503752660617E-02  .520133440431E-02  .537046882339E-02  .554510307185E-02  .572541599040E-02
   .591159223525E-02  .610382246712E-02  .630230354657E-02  .650723873558E-02  .671883790569E-02
   .693731775293E-02  .716290201977E-02  .739582172419E-02  .763631539635E-02  .788462932276E-02
   .814101779859E-02  .840574338805E-02  .867907719326E-02  .896129913194E-02  .925269822400E-02
   .955357288758E-02  .986423124464E-02  .101849914365E-01  .105161819495E-01  .108581419519E-01
   .112112216404E-01  .115757825996E-01  .119521981717E-01  .123408538391E-01  .127421476193E-01
   .131564904721E-01  .135843067208E-01  .140260344867E-01  .144821261375E-01  .149530487510E-01
   .154392845931E-01  .159413316118E-01  .164597039470E-01  .169949324574E-01  .175475652638E-01
   .181181683104E-01  .187073259445E-01  .193156415151E-01  .199437379906E-01  .205922585965E-01
   .212618674747E-01  .219532503631E-01  .226671152982E-01  .234041933402E-01  .241652393213E-01
   .249510326191E-01  .257623779547E-01  .266001062165E-01  .274650753115E-01  .283581710436E-01
   .292803080210E-01  .302324305924E-01  .312155138146E-01  .322305644506E-01  .332786220011E-01
   .343607597686E-01  .354780859567E-01  .366317448050E-01  .378229177610E-01  .390528246900E-01
   .403227251240E-01  .416339195521E-01  .429877507520E-01  .443856051652E-01  .458289143166E-01
   .473191562810E-01  .488578571964E-01  .504465928270E-01  .520869901769E-01  .537807291563E-01
   .555295443019E-01  .573352265534E-01  .591996250870E-01  .611246492098E-01  .631122703148E-01
   .651645238996E-01  .672835116512E-01  .694714035982E-01  .717304403333E-01  .740629353074E-01
   .764712771991E-01  .789579323611E-01  .815254473456E-01  .841764515121E-01  .869136597208E-01
   .897398751118E-01  .926579919768E-01  .956709987225E-01  .987819809310E-01  .101994124520E+00
   .105310719005E+00  .108735160869E+00  .112270957040E+00  .115921728481E+00  .119691213902E+00
   .123583273585E+00  .127601893339E+00  .131751188583E+00  .136035408556E+00  .140458940676E+00
   .145026315024E+00  .149742208992E+00  .154611452068E+00  .159639030781E+00  .164830093811E+00
   .170189957261E+00  .175724110099E+00  .181438219781E+00  .187338138056E+00  .193429906954E+00
   .199719764979E+00  .206214153496E+00  .212919723327E+00  .219843341560E+00  .226992098585E+00
   .234373315355E+00  .241994550880E+00  .249863609972E+00  .257988551235E+00  .266377695319E+00
   .275039633439E+00  .283983236179E+00  .293217662568E+00  .302752369466E+00  .312597121246E+00
   .322761999795E+00  .333257414835E+00  .344094114590E+00  .355283196787E+00  .366836120023E+00
   .378764715502E+00  .391081199148E+00  .403798184116E+00  .416928693710E+00  .430486174720E+00
   .444484511190E+00  .458938038641E+00  .473861558747E+00  .489270354497E+00  .505180205845E+00
   .521607405869E+00  .538568777456E+00  .556081690535E+00  .574164079857E+00  .592834463369E+00
   .612111961177E+00  .632016315122E+00  .652567909002E+00  .673787789445E+00  .695697687463E+00
   .718320040705E+00  .741678016440E+00  .765795535274E+00  .790697295655E+00  .816408799161E+00
   .842956376619E+00  .870367215068E+00  .898669385601E+00  .927891872115E+00  .958064600989E+00
   .989218471734E+00  .102138538864E+01  .105459829343E+01
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VASP 的 POTCAR


```
aepotential
  .249296618412E+05  .247076583257E+05  .244443255599E+05  .241414371172E+05  .238011681064E+05
  .234259054160E+05  .230182276498E+05  .225808680933E+05  .221166790321E+05  .216285959644E+05
  .211196020425E+05  .205926935296E+05  .200508469868E+05  .194969885786E+05  .189339660140E+05
  .183645234482E+05  .177912796436E+05  .172167095020E+05  .166431291099E+05  .160726841798E+05
  .155073419145E+05  .149488860093E+05  .143989147023E+05  .138588415092E+05  .133298984061E+05
  .128131411287E+05  .123094562646E+05  .118195698156E+05  .113440569063E+05  .108833523432E+05
  .104377617399E+05  .100074729506E+05  .959256758265E+04  .919303239296E+04  .880877039590E+04
  .843961154725E+04  .808532289425E+04  .774561810756E+04  .742016634235E+04  .710860038888E+04
  .681052409519E+04  .652551907131E+04  .625315067621E+04  .599297332353E+04  .574453513086E+04
  .550738195528E+04  .528106086162E+04  .506512306412E+04  .485912638819E+04  .466263730249E+04
  .447523256840E+04  .429650053920E+04  .412604216570E+04  .396347173509E+04  .380841738005E+04
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  .301689731751E+04  .290523647712E+04  .279862460324E+04  .269681368551E+04  .259956787532E+04
  .250666302499E+04  .241788621528E+04  .233303528113E+04  .225191833487E+04  .217435329790E+04
  .210016743837E+04  .202919692087E+04  .196128636819E+04  .189628843674E+04  .183406340726E+04
  .177447879164E+04  .171740895648E+04  .166273476188E+04  .161034321676E+04  .156012715054E+04
  .151198490272E+04  .146582002337E+04  .142154099431E+04  .137906095998E+04  .133829747604E+04
  .129917226882E+04  .126161100972E+04  .122554310047E+04  .119090147066E+04  .115762238690E+04
  .112564527212E+04  .109491253468E+04  .106536940758E+04  .103696379654E+04  .100964613669E+04
  .983369256582E+03  .958088251357E+03  .933760361363E+03  .910344858922E+03  .887802940737E+03
  .866097626532E+03  .845193663442E+03  .825057435693E+03  .805656879371E+03  .786961401872E+03
  .768941805860E+03  .751570217559E+03  .734820018832E+03  .718665782978E+03  .703083214326E+03
  .688049090980E+03  .673541210507E+03  .659538338921E+03  .646020162215E+03  .632967240499E+03
  .620360964749E+03  .608183515718E+03  .596417825223E+03  .585047539244E+03  .574056983177E+03
  .563431128839E+03  .553155563184E+03  .543216458754E+03  .533600545498E+03  .524295084194E+03
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  .474329191586E+03  .466879791201E+03  .459655261667E+03  .452646645612E+03  .445845314309E+03
  .439242952579E+03  .432831544450E+03  .426603359477E+03  .420550939758E+03  .414667087568E+03
  .408944853585E+03  .403377525679E+03  .397958618253E+03  .392681862072E+03  .387541194587E+03
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  .359239359657E+03  .354897094389E+03  .350648839276E+03  .346490025719E+03  .342416217091E+03
  .338423103118E+03  .334506494502E+03  .330662317854E+03  .326886610852E+03  .323175517677E+03
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  .254279729706E+03  .251186798183E+03  .248091905310E+03  .244992928548E+03  .241887803987E+03
  .238774526866E+03  .235651152274E+03  .232515796051E+03  .229366635883E+03  .226201912602E+03
  .223019931688E+03  .219819064985E+03  .216597752635E+03  .213354505238E+03  .210087906247E+03
  .206796614606E+03  .203479367655E+03  .200134984304E+03  .196762368500E+03  .193360513013E+03
  .189928503567E+03  .186465523338E+03  .182970857876E+03  .179443900479E+03  .175884158076E+03
  .172291257693E+03  .168664953559E+03  .165005134953E+03  .161311834879E+03  .157585239680E+03
  .153825699735E+03  .150033741355E+03  .146210080040E+03  .142355635261E+03  .138471546918E+03
  .134559193631E+03  .130620212984E+03  .126656523815E+03  .122670350542E+03  .118664249404E+03
  .114641136335E+03  .110604315898E+03  .106557510391E+03  .102504887754E+03  .984510863142E+02
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  .744246633582E+02  .705324162159E+02  .666918555610E+02  .629102856287E+02  .591944669183E+02
  .555502477826E+02  .519821532120E+02  .484929672536E+02  .450833747318E+02  .417517679306E+02
  .384943726247E+02  .353058986338E+02  .321809414460E+02  .291163276325E+02  .261144334538E+02
  .231871492547E+02  .203596538297E+02  .176726025177E+02  .151810751243E+02  .129490421749E+02
  .110393419236E+02  .950085943829E+01  .835601596774E+01  .759220035195E+01  .716026979128E+01
  .698171586735E+01  .696337537316E+01  .701521042419E+01  .706481632887E+01  .706399956522E+01
  .698712622280E+01  .682461424434E+01  .657568967629E+01  .624298209986E+01  .582958804938E+01
  .533805380599E+01  .477041519949E+01  .412860165824E+01  .341481131402E+01  .263171136544E+01
  .178246368857E+01  .870634878579E+00 -.999438728779E-01 -.112531868169E+01 -.220152969452E+01
 -.332469269108E+01 -.449104609659E+01 -.569696875391E+01 -.693897492955E+01 -.821369210611E+01
 -.951782536530E+01 -.108481102767E+02 -.122012545007E+02 -.135738669876E+02 -.149623728146E+02
 -.163629115444E+02 -.177712178383E+02 -.191824854283E+02 -.205912200739E+02 -.219910944781E+02
 -.233748284178E+02 -.247341312735E+02 -.260597521130E+02 -.273417019240E+02 -.285696929862E+02
 -.297338408481E+02 -.308256300402E+02 -.318391145291E+02 -.327722934381E+02 -.336286096960E+02
 -.344184453032E+02 -.351602594335E+02 -.358801411316E+02 -.366068307978E+02 -.373574862777E+02
 -.381118849160E+02 -.387867273418E+02 -.392441857634E+02 -.393634904186E+02 -.391349287009E+02
 -.386756216504E+02 -.381417407639E+02 -.376357898778E+02 -.371876084285E+02 -.367857308718E+02
 -.364089017521E+02 -.360404072746E+02 -.356705440643E+02 -.352947736909E+02 -.349113812250E+02
 -.345198086599E+02 -.341197549222E+02 -.337108274651E+02
```

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  .566100405752E-04  .603274790726E-04  .642889041986E-04  .685103164325E-04  .730087642691E-04
  .778024127357E-04  .829106163764E-04  .883539969928E-04  .941545264508E-04  .100335614880E-03
  .106922204616E-03  .113940870262E-03  .121419925256E-03  .129389535376E-03  .137881839620E-03
  .146931078955E-03  .156573733420E-03  .166848668143E-03  .177797288839E-03  .189463707397E-03
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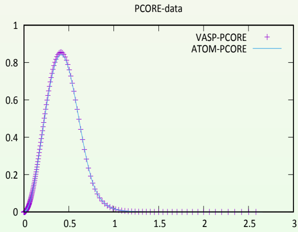

VASP 的 POTCAR


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  .795189540556E+01   .806575163262E+01   .818409040251E+01   .830711427710E+01   .843503666033E+01
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VASP 的 POTCAR


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 -.285135138679E+02  -.285135676456E+02  -.285136239791E+02  -.285136830688E+02  -.285137451272E+02
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 -.285162971590E+02  -.285165174159E+02  -.285167517787E+02  -.285170011938E+02  -.285172666691E+02
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VASP 的 POTCAR


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core charge-density (pseudized)
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  .301257706327E-07  .321168550529E-07  .342395350151E-07  .365025079838E-07  .389150462599E-07
  .414870349726E-07  .442290125832E-07  .471522140648E-07  .502686169368E-07  .535909903417E-07
  .571329473648E-07  .609090008129E-07  .649346226787E-07  .692263075359E-07  .738016401239E-07
  .786793673994E-07  .838794753501E-07  .894232708855E-07  .953334691390E-07  .101634286542E-06
  .108351540046E-06  .115512752907E-06  .123147267460E-06  .131286365342E-06  .139963395669E-06
  .149213911678E-06  .159075816404E-06  .169589517985E-06  .180798095227E-06  .192747474115E-06
  .205486615992E-06  .219067718171E-06  .233546427810E-06  .248982069915E-06  .265437890425E-06
  .282981315349E-06  .301684227038E-06  .321623258718E-06  .342880108482E-06  .365541874040E-06
  .389701409594E-06  .415457706293E-06  .442916297843E-06  .472189692914E-06  .503397836133E-06
  .536668599544E-06  .572138306547E-06  .609952290465E-06  .650265490033E-06  .693243084236E-06
  .739061169114E-06  .787907479286E-06  .839982157176E-06  .895498573063E-06  .954684199344E-06
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  .140161500606E-05  .149425104883E-05  .159300962235E-05  .169829537834E-05  .181053971277E-05
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  .694222925437E-05  .740105648627E-05  .789020852588E-05  .841168958728E-05  .896763634441E-05
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VASP 的 POTCAR


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VASP 的 POTCAR


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VASP 的 POTCAR


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VASP 的 POTCAR


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VASP 的 POTCAR

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VASP 的 POTCAR


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VASP 的 POTCAR


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End of Dataset
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谢谢大家！