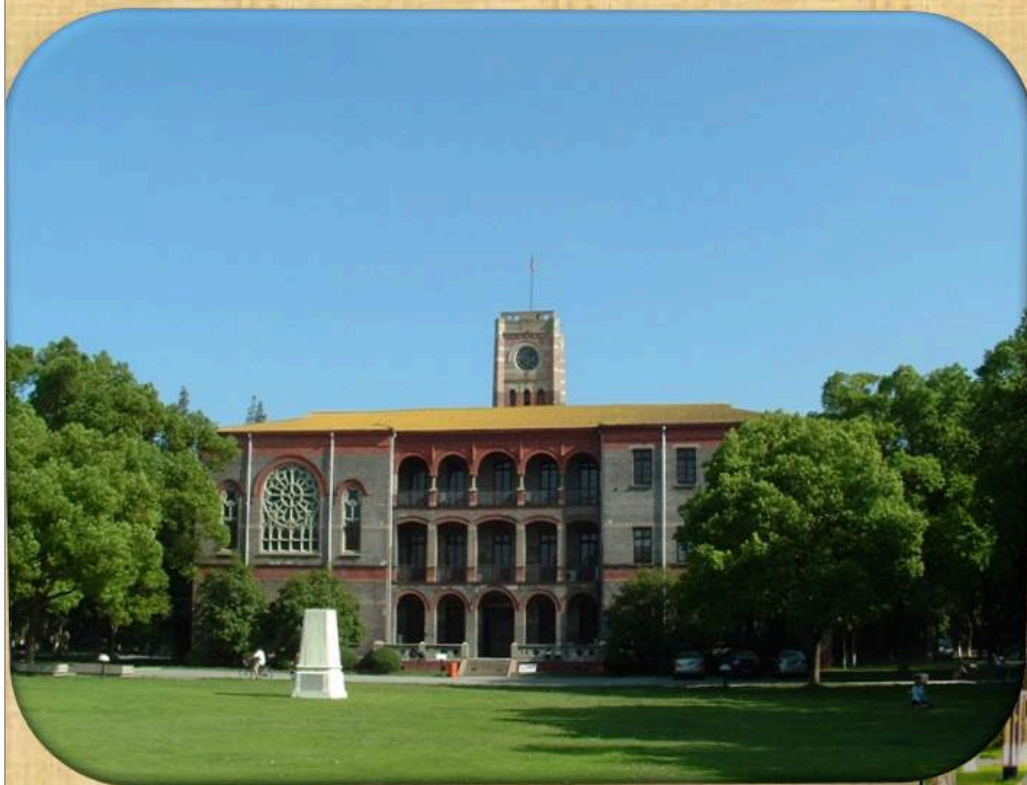




结构化学习题参考答案



2025/4/9





1. (1) 写出 Na^+ 与 F^- 的薛定谔方程
(2) 写出哈特里自洽场下的单电子薛定谔方程。

答: Na^+ : 10个电子, $Z=11$

$$\left[\sum_{i=1}^{10} \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right) - \sum_{i=1}^{10} \frac{11 e^2}{4\pi \epsilon_0 r_i} + \frac{1}{2} \sum_{i=1}^{10} \sum_{j \neq i} \frac{e^2}{4\pi \epsilon_0 r_{ij}} \right] \Psi = E \Psi$$

$$\text{或 } \sum_{i=1}^9 \sum_{j>i+1}^{10} \frac{e^2}{4\pi \epsilon_0 r_{ij}}$$



F⁻ : 10个电子, Z=9

$$\left[\sum_{i=1}^{10} \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right) - \sum_{i=1}^{10} \frac{9 e^2}{4\pi \epsilon_0 r_i} + \frac{1}{2} \sum_{i=1}^{10} \sum_{j \neq i} \frac{e^2}{4\pi \epsilon_0 r_{ij}} \right] \Psi = E \Psi$$

哈特里自洽场单电子薛定谔方程:

$$\left(-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} + \sum_{j \neq i}^{N-1} \int \frac{1}{r_{ij}} |\varphi_j|^2 d\tau_j \right) \varphi_i = E_i \varphi_i$$

其中: Na⁺ : Z=11, N=10;

F⁻ : Z=9, N=10;



13. 试写出Be原子的激发态($1s^2 2s^1 2p^1$)的Slater行列式波函数。

解：设该激发态的电子排布为：

1s	2s	2p		
$\begin{array}{ c } \hline \uparrow\downarrow \\ \hline \end{array}$	$\begin{array}{ c } \hline \uparrow \\ \hline \end{array}$	$\begin{array}{ c } \hline \\ \hline \end{array}$	$\begin{array}{ c } \hline \downarrow \\ \hline \end{array}$	$\begin{array}{ c } \hline \\ \hline \end{array}$
		m=-1	0	1

其Slater行列式波函数为：

$$\Psi = \frac{1}{\sqrt{4!}} \begin{vmatrix} 1s(1)\alpha(1) & 1s(2)\alpha(2) & 1s(3)\alpha(3) & 1s(4)\alpha(4) \\ 1s(1)\beta(1) & 1s(2)\beta(2) & 1s(3)\beta(3) & 1s(4)\beta(4) \\ 2s(1)\alpha(1) & 2s(2)\alpha(2) & 2s(3)\alpha(3) & 2s(4)\alpha(4) \\ 2p_0(1)\beta(1) & 2p_0(2)\beta(2) & 2p_0(3)\beta(3) & 2p_0(4)\beta(4) \end{vmatrix}$$