



$\text{Li}_2$  molecule

$$\begin{aligned}
 \hat{H} = & -\frac{\hbar^2}{2m_A} \frac{\partial^2}{\partial \vec{R}_A^2} - \frac{\hbar^2}{2m_B} \frac{\partial^2}{\partial \vec{R}_B^2} + \frac{z_A z_B e^2}{4\pi\epsilon_0 |\vec{R}_A - \vec{R}_B|} \\
 & - \frac{\hbar^2}{2m_e} \sum_{i=1}^6 \frac{\partial^2}{\partial \vec{r}_i^2} - \frac{z_A e^2}{4\pi\epsilon_0} \sum_{i=1}^6 \frac{1}{|\vec{R}_A - \vec{r}_i|} - \frac{z_B e^2}{4\pi\epsilon_0} \sum_{i=1}^6 \frac{1}{|\vec{R}_B - \vec{r}_i|} \\
 & + \frac{e^2}{4\pi\epsilon_0} \sum_{i=1}^6 \sum_{j=1}^{i-1} \frac{1}{|\vec{r}_i - \vec{r}_j|} .
 \end{aligned}$$

$$z_A = z_B = 3$$