$$H_{i,i} = \begin{pmatrix} \varepsilon_s & 0 & 0 & 0 \\ 0 & \varepsilon_p & 0 & 0 \\ 0 & 0 & \varepsilon_p & 0 \\ 0 & 0 & 0 & \varepsilon_p \end{pmatrix}$$

$$H_{i,j} = \begin{pmatrix} h_{s^i s^j} & h_{s^i p_x^j} & h_{s^i p_y^j} & h_{s^i p_z^j} \\ h_{p_x^i s^j} & h_{p_x^i p_x^j} & h_{p_x^i p_y^j} & h_{p_x^i p_z^j} \\ h_{p_y^i s^j} & h_{p_y^i p_x^j} & h_{p_y^i p_y^j} & h_{p_y^i p_z^j} \\ h_{p_z^i s^j} & h_{p_z^i p_x^j} & h_{p_z^i p_y^j} & h_{p_z^i p_z^j} \end{pmatrix}$$

$$h_{\alpha^i,\beta^j} = \sum_i^N \sum_{j\neq i}^N \mu_{\alpha^i,\beta^j}(|(r_j - r_i)|)\exp[ik.(r_j - r_i)]$$

Is the hooping integral between the orbital α of the atom i and the orbital β of the atom j. the expression for μ_{α^i,β^j} is shown in the following table:

	s^j	p_x^j	p_y^j	p_z^j
s^i	$v_{ss\sigma}$	$lv_{sp\sigma}$	$mv_{sp\sigma}$	$nv_{sp\sigma}$
p_x^i	$-lv_{sp\sigma}$	$l^2 v_{pp\sigma} + (1 - l^2)v_{pp\pi}$	$lm(v_{pp\sigma} - v_{pp\pi})$	$\ln((v_{pp\sigma} - v_{pp\pi})$
p_y^i	$-mv_{sp\sigma}$	$lm(v_{pp\sigma} - v_{pp\pi})$	$m^2 v_{pp\sigma} + (1 - m^2)v_{pp\pi}$	$mn(v_{pp\sigma} - v_{pp\pi})$
p_z^i	$-nv_{sp\sigma}$	$\ln((v_{pp\sigma} - v_{pp\pi})$	$mn(v_{pp\sigma} - v_{pp\pi})$	$n^2 v_{pp\sigma} + (1 - n^2)v_{pp\pi}$

Here $l = (r_j - r_i).\hat{X}$ $m = (r_j - r_i).\hat{Y}$ $n = (r_j - r_i).\hat{Z}$