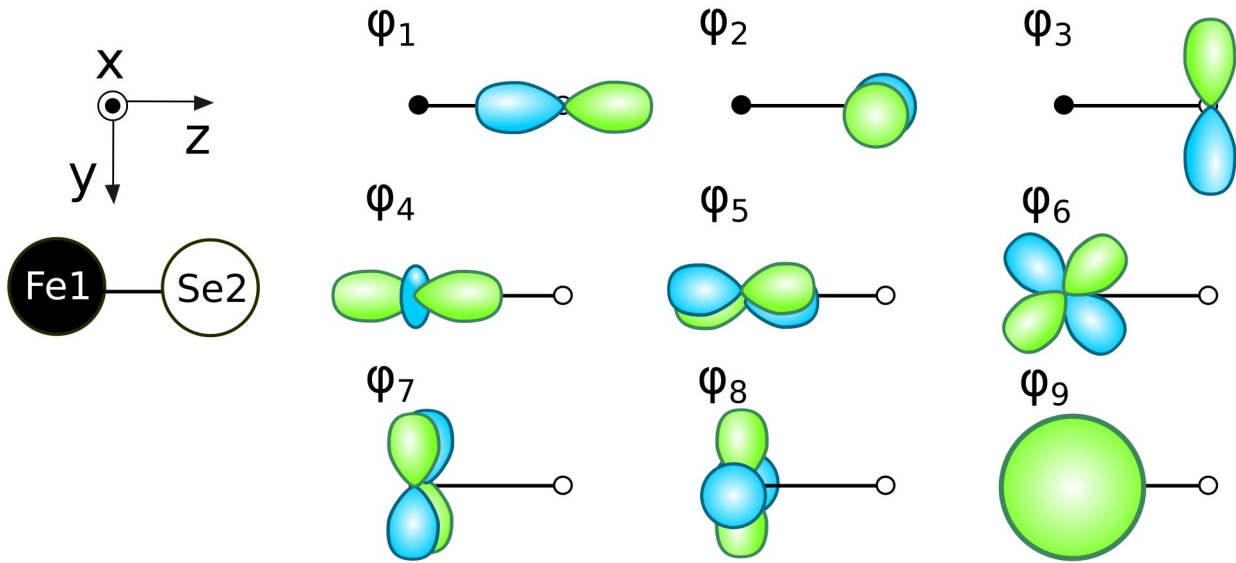


# Model Hamiltonian for the FeSe molecule

Localized orbitals:



Model:

$$H = E_0 + \sum_i \varepsilon_i n_i + \sum_{i,j,\eta} t_{ij} c_{i,\eta}^\dagger c_{j,\eta} + \text{h.c.} + \sum_i U_i n_{i,\uparrow} n_{i,\downarrow} + \sum_{i,j} V_{ij} n_i n_j + \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

Orbital energies ( $n_i = c_i^\dagger c_i$ )

$$\varepsilon s \ n_{\varphi 9}$$

$$\varepsilon p \sigma \ n_{\varphi 1}$$

$$\varepsilon p \pi \ (n_{\varphi 2} + n_{\varphi 3})$$

$$\varepsilon d \sigma \ n_{\varphi 4}$$

$$\varepsilon d \pi \ (n_{\varphi 5} + n_{\varphi 6})$$

$$\varepsilon d \delta \ (n_{\varphi 7} + n_{\varphi 8})$$

$$\varepsilon d \ (n_{\varphi 4} + n_{\varphi 5} + n_{\varphi 6} + n_{\varphi 7} + n_{\varphi 8})$$

$$\varepsilon p \ (n_{\varphi 1} + n_{\varphi 2} + n_{\varphi 3})$$

Symmetry-allowed hoppings

$$t \sigma \ \sum_{\eta} (c_{\varphi 1,\eta}^\dagger c_{\varphi 4,\eta} + \text{h.c.})$$

$$t \sigma p \ \sum_{\eta} (c_{\varphi 1,\eta}^\dagger c_{\varphi 9,\eta} + \text{h.c.})$$

$$t \sigma a l l \ \sum_{\eta} (c_{\varphi 1,\eta}^\dagger c_{\varphi 4,\eta} + c_{\varphi 1,\eta}^\dagger c_{\varphi 9,\eta} + \text{h.c.})$$

$$t \pi \ \sum_{\eta} (c_{\varphi 2,\eta}^\dagger c_{\varphi 5,\eta} + c_{\varphi 3,\eta}^\dagger c_{\varphi 6,\eta} + \text{h.c.})$$

$$t \ \sum_{\eta} (c_{\varphi 1,\eta}^\dagger c_{\varphi 4,\eta} + c_{\varphi 1,\eta}^\dagger c_{\varphi 9,\eta} + c_{\varphi 2,\eta}^\dagger c_{\varphi 5,\eta} + c_{\varphi 3,\eta}^\dagger c_{\varphi 6,\eta} + \text{h.c.})$$

Self-repulsion

$$U p \ (n_{\varphi 1,\uparrow} n_{\varphi 1,\downarrow} + n_{\varphi 2,\uparrow} n_{\varphi 2,\downarrow} + n_{\varphi 3,\uparrow} n_{\varphi 3,\downarrow})$$

$$U d \sigma \ n_{\varphi 4,\uparrow} n_{\varphi 4,\downarrow}$$

$$U d \pi \ (n_{\varphi 5,\uparrow} n_{\varphi 5,\downarrow} + n_{\varphi 6,\uparrow} n_{\varphi 6,\downarrow})$$

$$U d \delta \ (n_{\varphi 7,\uparrow} n_{\varphi 7,\downarrow} + n_{\varphi 8,\uparrow} n_{\varphi 8,\downarrow})$$

$$U d \ \sum_{i=4}^8 n_{\varphi i,\uparrow} n_{\varphi i,\downarrow}$$

$$U \ \sum_{i=1}^9 n_{\varphi i,\uparrow} n_{\varphi i,\downarrow}$$

Couloumb interaction

$$V p d \ \sum_{i=1}^3 \sum_{j=4}^8 n_{\varphi i} n_{\varphi j}$$

$$V p s \ \sum_{i=1}^9 n_{\varphi i} n_{\varphi 9}$$

Exchange

$$J \ \sum_{i=4}^8 \sum_{j>i} S_{\varphi i} S_{\varphi j}$$