

# Hosts, hybrids, and caps [pln11]

Here we generalize [pln10] to also permit triple occupancy of orbitals.

The first particle placed into an orbital belongs to the *host* category. The second particle placed into the same orbital is being hosted and can host another particle. It belongs to the *hybrid* category. The third particle placed is being hosted (by a hybrid) and cannot host further particles. It belongs to the *cap* category.

Hosts, hybrids, and caps have activation energies  $\epsilon_1, \epsilon_2, \epsilon_3$ , respectively.

Multiplicity of microstates with  $N_1$  hosts,  $N_2$  hybrids, and  $N_3$  caps:

$$W(\{N_m\}) = \prod_{m=1}^3 \binom{d_m + N_m - 1}{N_m}, \quad d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}),$$

$$\mathbf{g} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}, \quad A_1 = N_A, \quad A_2 = A_3 = 0.$$

We encode the state of each orbital as vacant (0), occupied by a host (1), by a host and a hybrid (2), or by host, a hybrid, and a cap (3).

Microstates for  $N_A = 2$ :

00  
10 01  
20 02, 11  
30 03, 21 12  
31 13, 22  
32 23  
33

Microstates for  $N_A = 3$ :

000  
100 010 001  
110 101 011, 200 020 002  
111, 210 201 021 120 102 012, 300 030 003  
211 121 112, 220 202 022, 310 301 031 130 103 013  
221 212 122, 311 131 113, 320 302 032 230 203 023  
222, 321 213 132 312 123 231, 330 303 033  
322 232 223, 331 313 133  
332 323 233  
333