

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