where and denote the occupation of the *m* sublevel of spin , and the occupation of the host material without doping. The parameter can be tuned to fulfil the linearity of $E(N)$, i.e., the generalized Koopmans condition:

$$\Delta_{nk} = E(N\text{-}1) - E(N) + eig(N) = 0, \quad (2)$$

where $E(N\text{-}1) - E(N)$ denotes the total energy cost to rem