

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

$$n_k = E(N-1) - E(N) + \epsilon_{\text{ig}}(N) = 0, \quad (2)$$

where $E(N-1) - E(N)$ denotes the total energy cost to rem