

## Supporting information

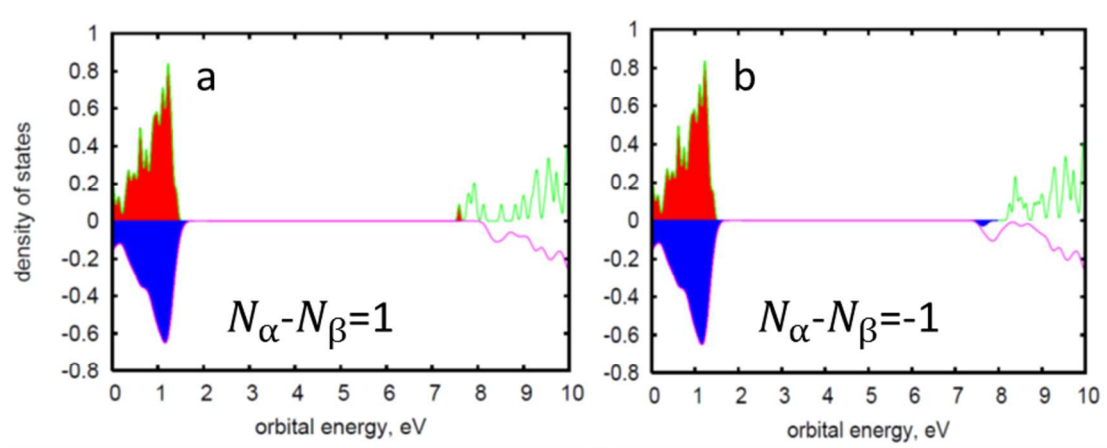
### DFT Calculation of Russell-Saunders Splitting for Lanthanide Ions Doped in Hexagonal ( $\beta$ ) - NaYF<sub>4</sub> Nanocrystals

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Ce<sup>3+</sup> has solo f-f transition from  $^2F_{5/2} \rightarrow ^2F_{7/2}$ . The comparison of spin flip shows only 0.01eV changing in total energy shown below. The swap of majority and minority spin components do not affect observables.



DOS of Na<sub>24</sub>Y<sub>23</sub>Ce<sub>1</sub>F<sub>96</sub> when the f electron at (a) spin( $\alpha$ ) and (b) spin( $\beta$ )