Electronic Supplementary Material (ESI) for RSC Advances.

Fig. S1 (a) density of states of a neutral V_{Zn} in the ZnS nanoparticle model calculated by PBE functional, showing the fermi level E_F pinning at around 1/3 of the defect spin down states; (b) spin density map (isosurface value = $3\times10^{-3}e/Å^3$) of the corresponding V_{Zn} calculated by PBE functional. The pink, blue and purple balls represent the pseudohydrogen, S and Zn atoms, respectively.

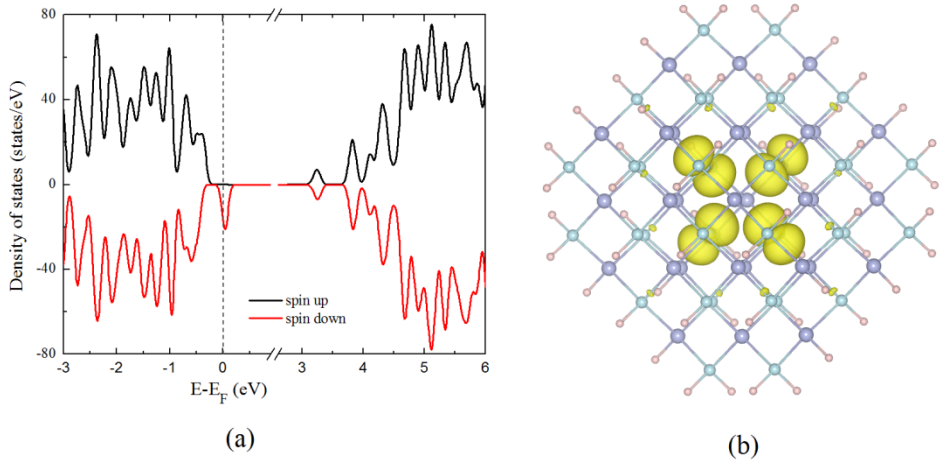

Fig. S2 Spin density distribution (8×10^{-3} $e/Å^3$) of V_{Zn}^0 in a 64-atom ZnS supercell calculated by HSE06 with an amount of the Hartree-Fock exchange (a) α = 0. 25 and (b) α = 0.35. The defect structure was relaxed with α = 0.25 by default. The small and large balls represent S and Zn atoms.