Supporting Information

Effects of intrinsic defects and extrinsic doping on the electronic and photocatalytic properties of Ta_3N_5

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Correction for the image charge interactions

Due to the limited size of the supercell, the correction for image charge interactions is include in the defect formation energy calculation, and only the corrections for defects with high charge states, i.e. N_{V3}, N_{V4} and Ta_i, are taken into account, since the image charge interaction is small for the other defects with low charge states. To estimate the magnitude and decay behavior of this interactions, the supercells containing 96, 128, 160 and 384 atoms are employed, and the formation energies of these defects are plotted as a function of L^{-1}, where L is the cube root of the corresponding supercell volume. We note that the defect formation energies are not linear with L-1, indicating that the elastic interaction may make a considerable contribution to them. However, the formation energies achieve a good convergence when the atom number of supercell reaches 384. Therefore, the 384 atom supercell is adopted to correct the defect formation energies of N_{V3}, N_{V4} and Ta_i.

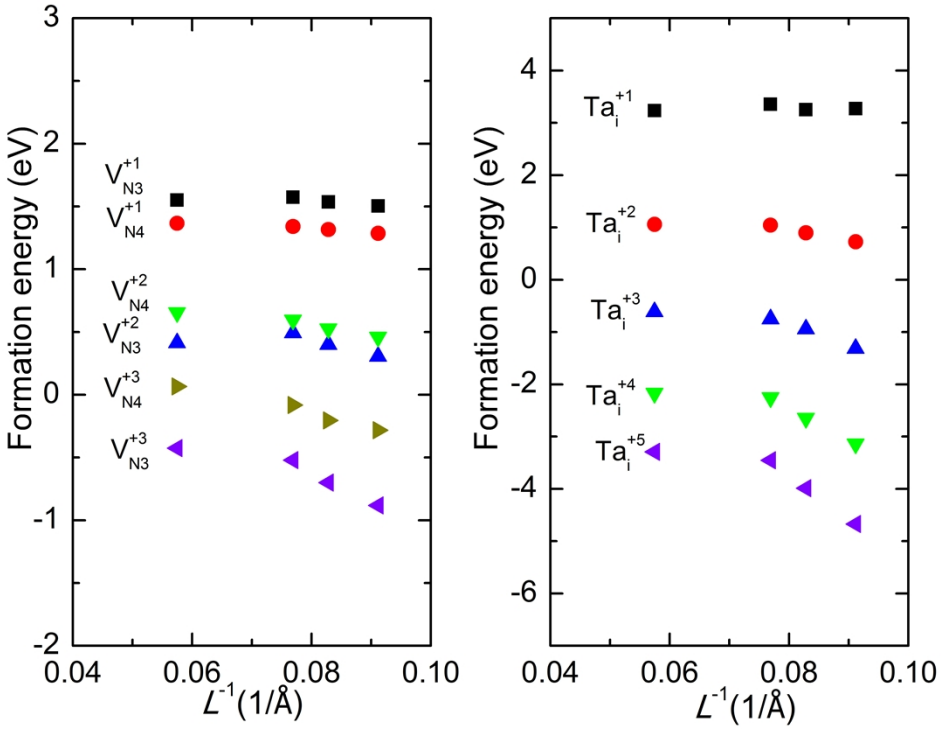

Figure S1 The defect formation energies of N_{V3}, N_{V4} and Ta_i as a function of supercell size.

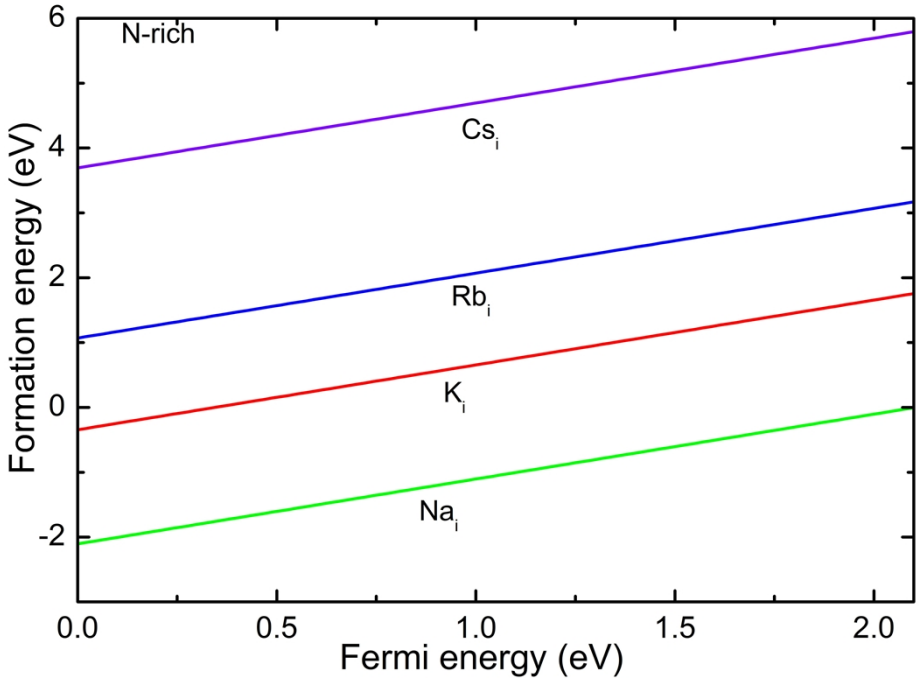

Figure S2 Calculated formation energies of defects as a function of the Fermi energy of

alkali metal interstitial doped Ta_3N_5 under N-rich condition.

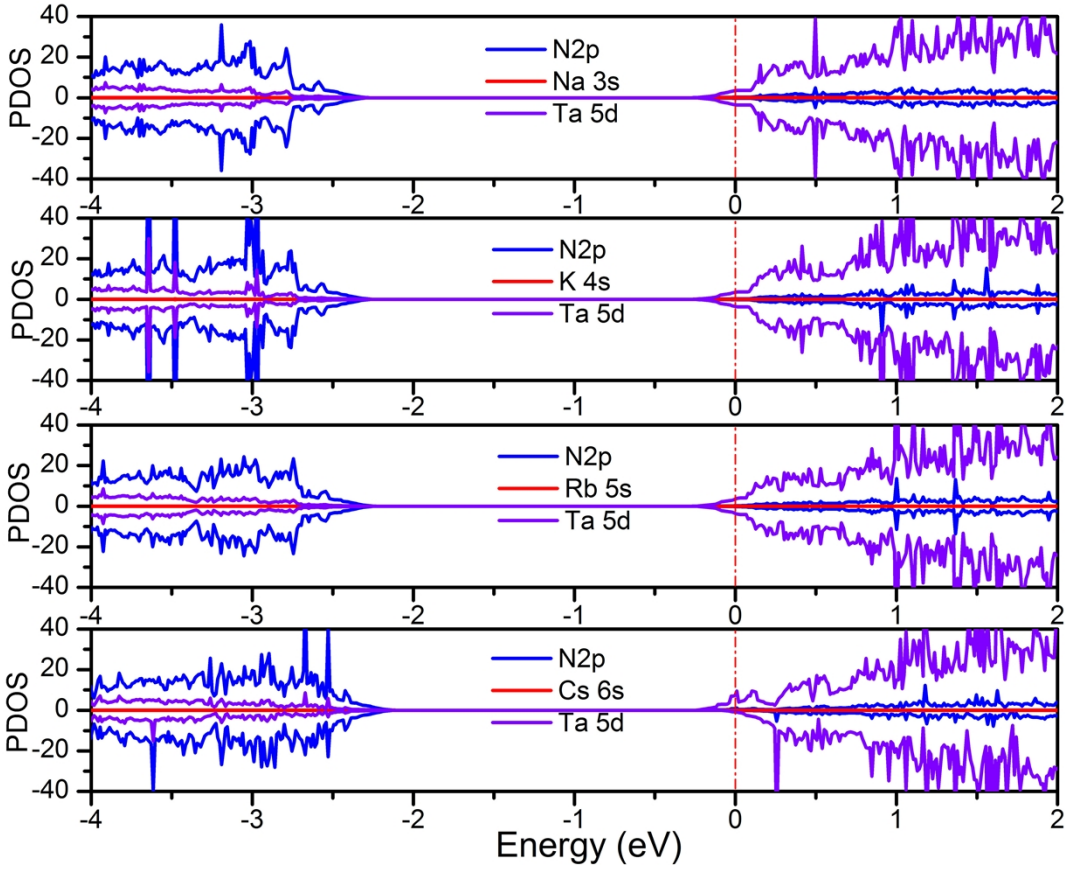

Figure 3 Calculated projected density of states (PDOS) for interstitial Na (a), K (b), Rb (c) and Cs (d) doped Ta_3N_5.