Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for:

Effect of Ni cocatalyst on photocatalytic hydrogen evolution reaction of anatase TiO_2 by first-principles calculations

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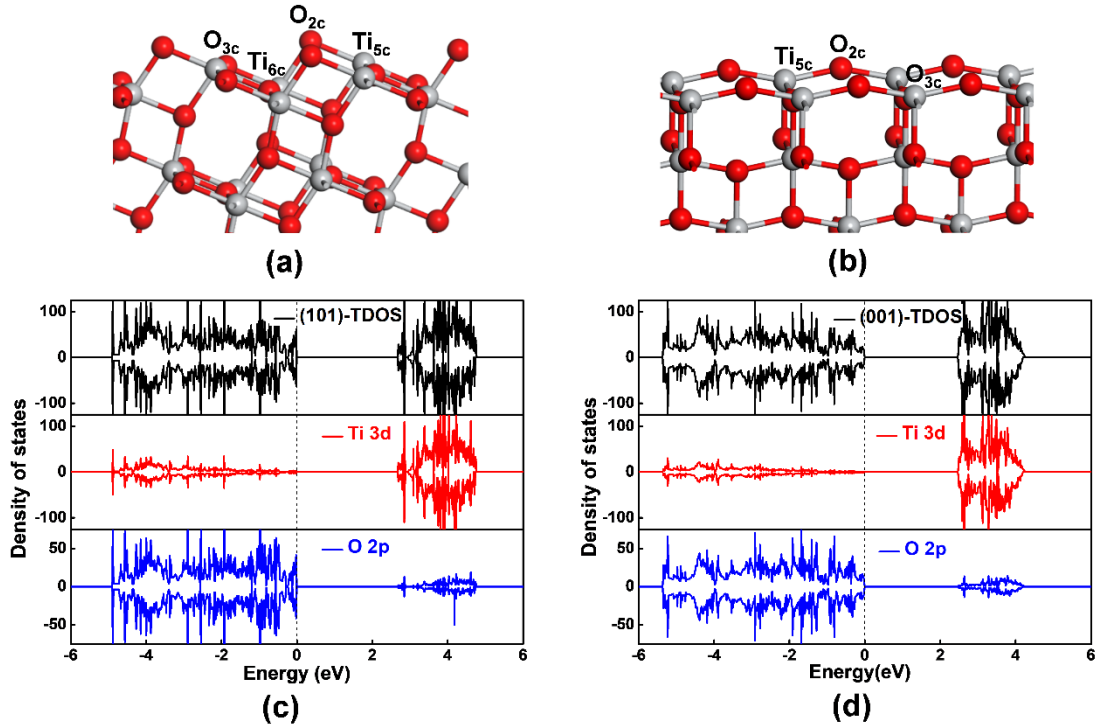

Fig. S1 The structures of (a) (101) and (b) (001) surfaces of anatase TiO_2. Coloring scheme: red balls (O) and gray balls (Ti).Calculated density of states for (c) (101) and (d) (001) surfaces.

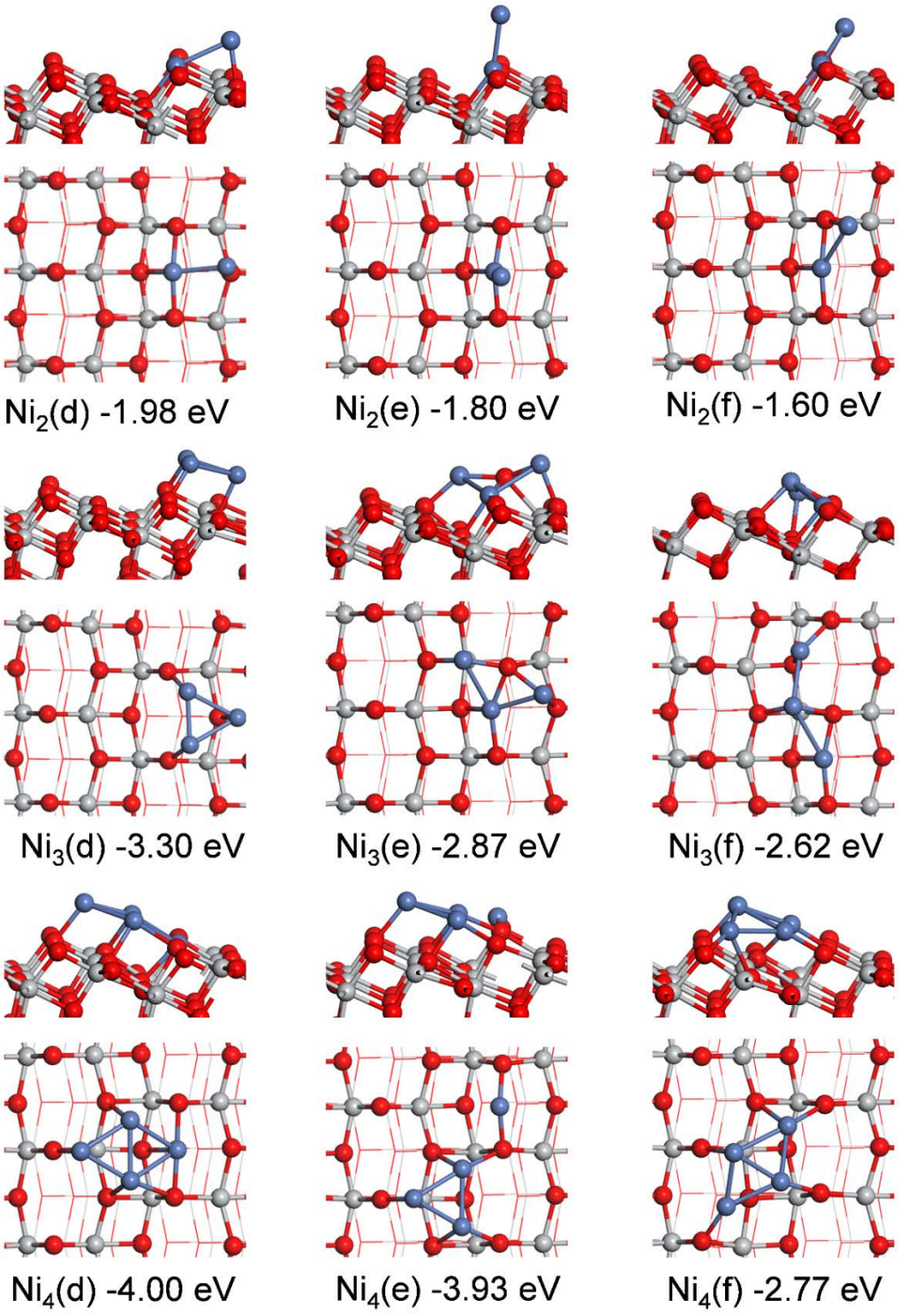

Fig. S2. Other optimized structures of $Ni_n/TiO_2(101)$ (n=1-4) (side and top views). Adsorption energies are shown below structures. Coloring scheme: red (O), gray (Ti) and blue (Ni).

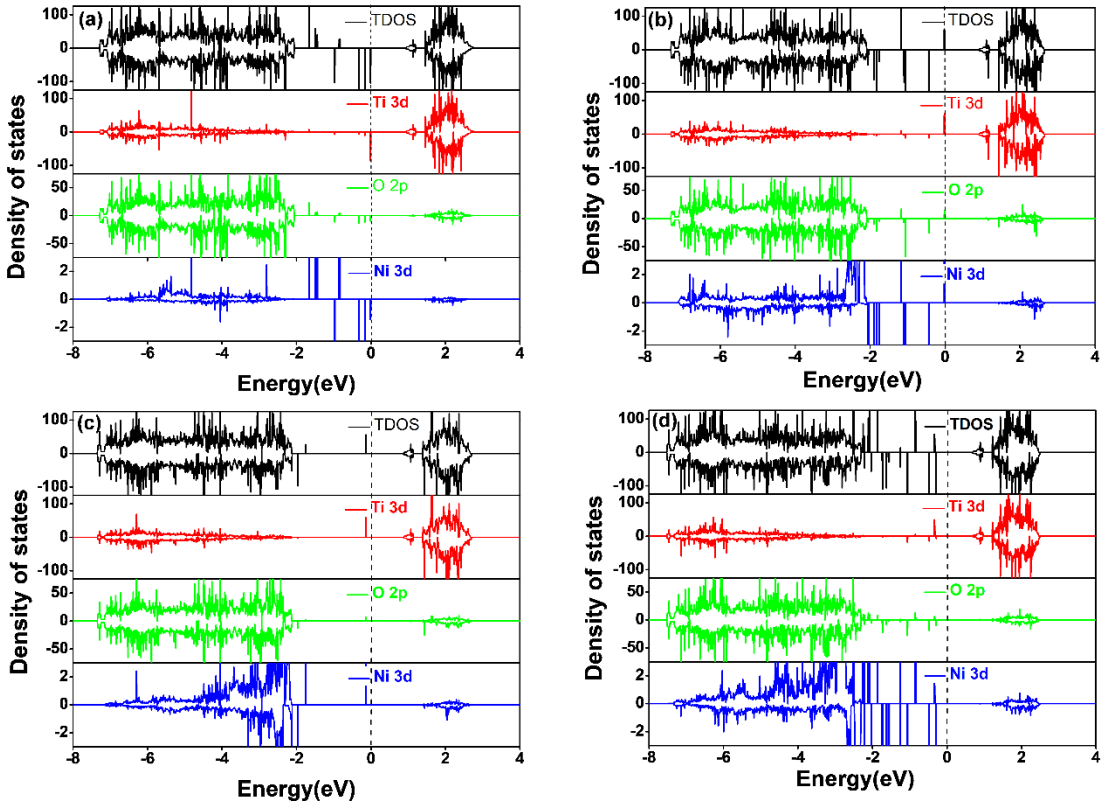

Fig. S3 Density of states for the most stable structure of (a) Ni, (b) Ni_2, (c) Ni_3, (d) Ni_4 adsorbed on TiO_2(101) surface calculated by HSE06 method. The Fermi level is shown by the vertical dashed line.

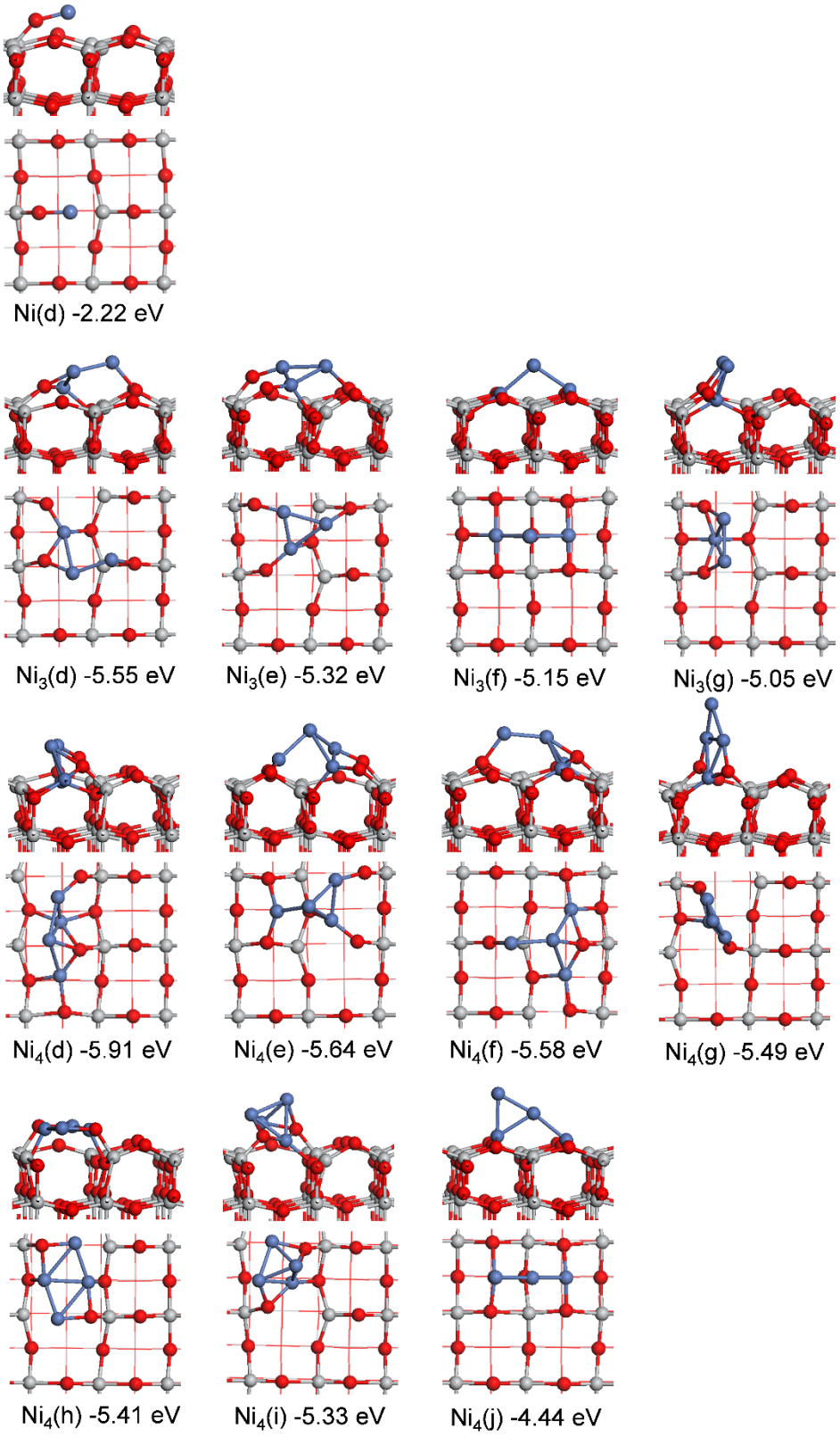

Fig. S4. Other optimized structures of $Ni_n/TiO_2(001)$ (n=1-4) (side and top views). Adsorption energies are shown below structures. Coloring scheme: red (O), gray (Ti) and blue (Ni).