

## Supporting Information for:

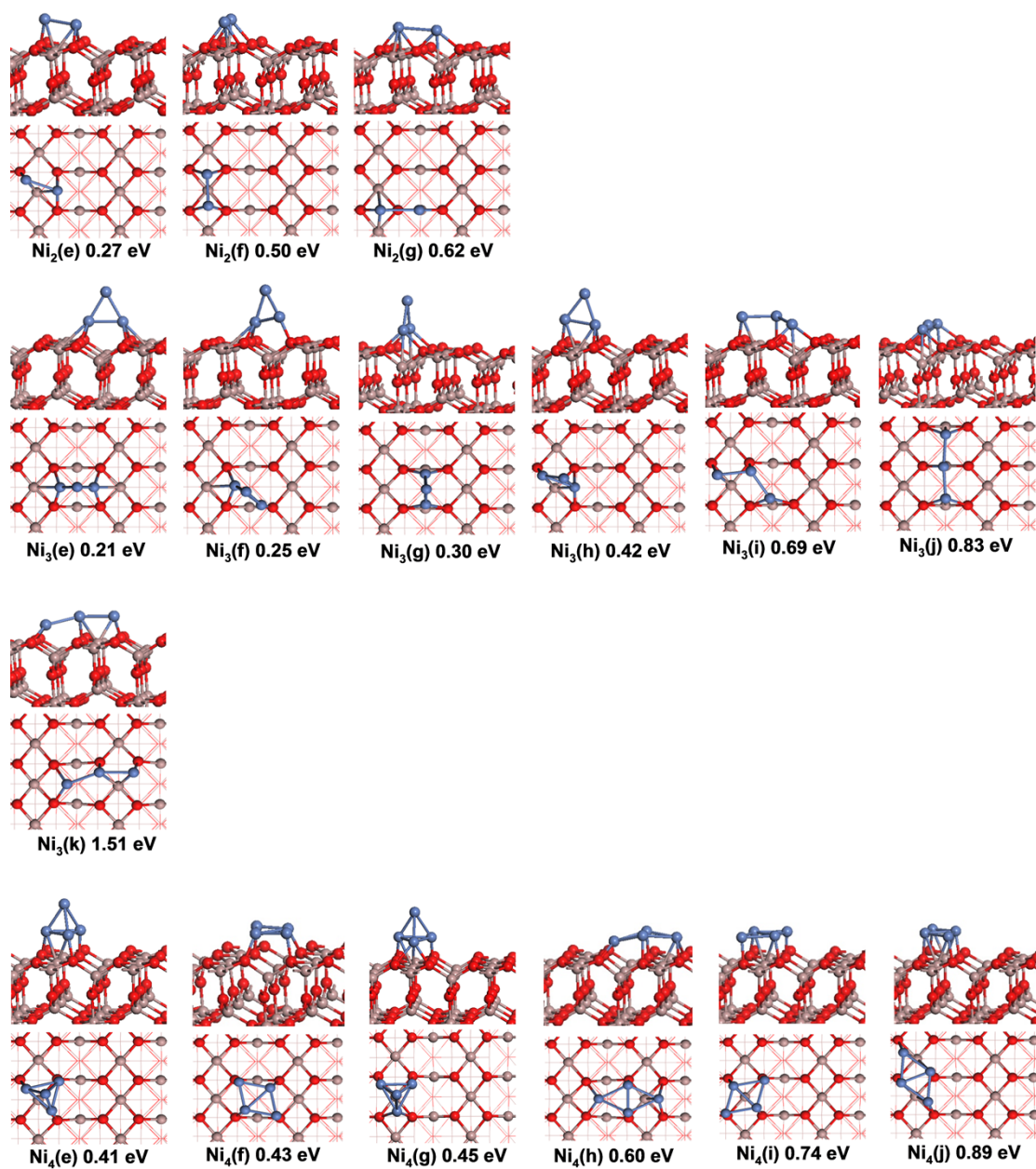
### Theoretical insight into the roles of cocatalysts in Ni-NiO/ $\beta$ - $\text{Ga}_2\text{O}_3$ photocatalyst for overall water splitting

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**Figure S1.** Less stable configurations of Ni<sub>n</sub>/Ga<sub>2</sub>O<sub>3</sub>(100) (n=1-4) clusters (side and top views). Relative energies with respect to the corresponding lowest-energy structure are shown. Coloring scheme: red (surface O), brown (Ga) and blue (Ni).



**Figure S2.** Less stable configurations of  $\text{Ni}_n\text{O}_n/\text{Ga}_2\text{O}_3(100)$  ( $n=1-4$ ) clusters (side and top views). Relative energies with respect to the corresponding lowest-energy structure are shown. Coloring scheme: red (surface O), brown (Ga), yellow (adsorbed O) and blue (Ni).