Supporting Information

Interface Effects in Hydrogen Elimination Reaction from Isopropanol by Ni_{13} Cluster on Θ-Al_2O_3(010) Surface

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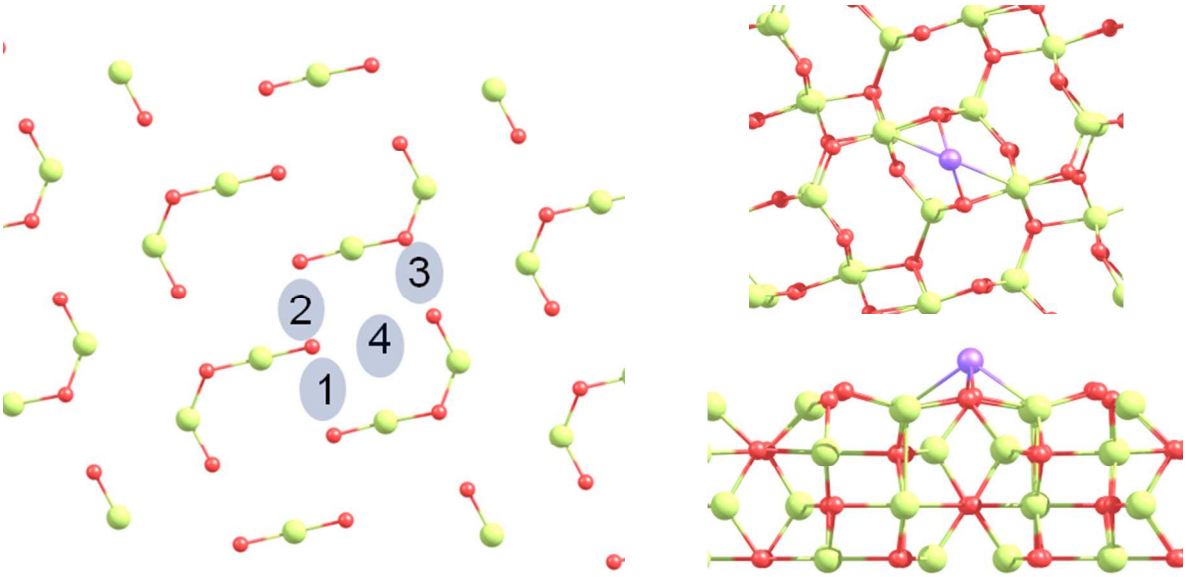
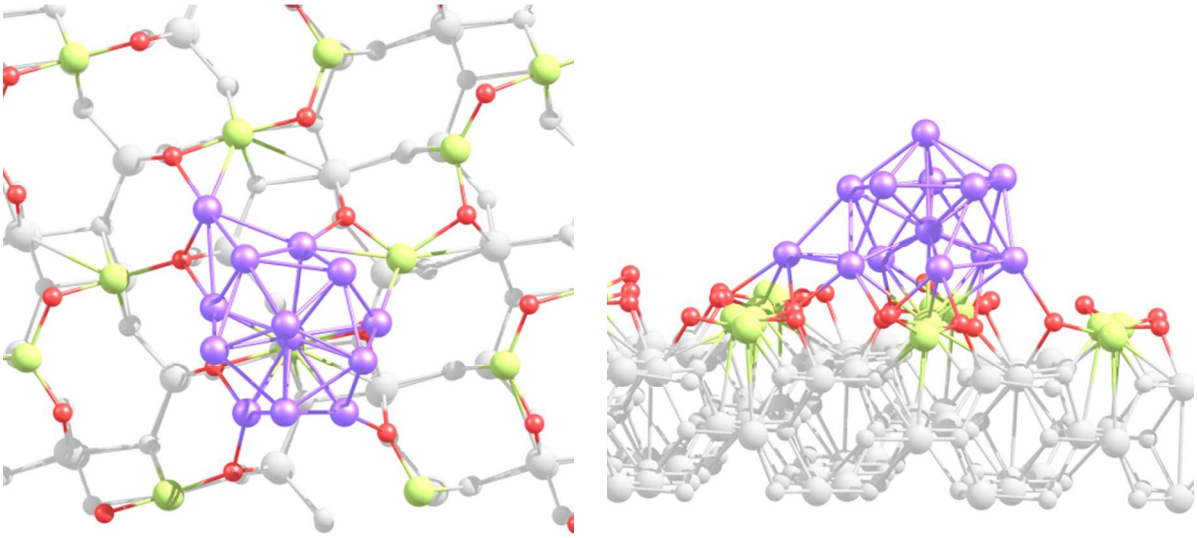


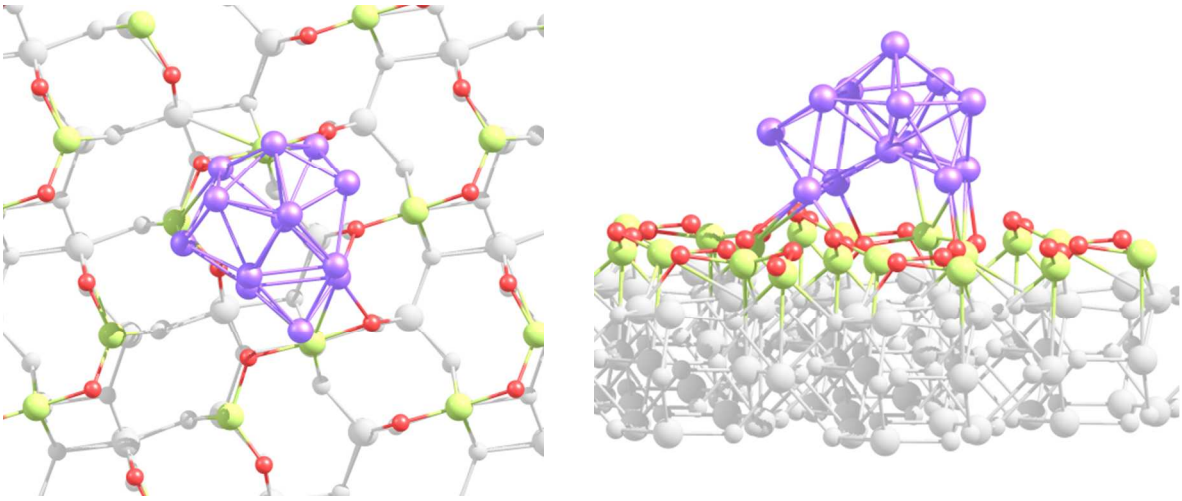
Figure S1 Left: Schematic representation of the most favorable adsorption sites of a single Ni atom on θ-Al_2O_3(010) surface with the binding energy E_b: (1) E_b=3.16 eV; (2) E_b=3.09 eV; (3) E_b=2.97 eV; (4) E_b=2.67 eV. Only first atomic layer of θ-Al_2O_3(010) is shown. Ni prefers to bridge the low coordinated O atoms on the θ-Al_2O_3(010) surface. Right: Optimized the most stable geometry of Ni on θ-Al_2O_3(010) surface. Aluminum atoms are yellow-green-colored and oxygen atoms are red-colored.

a)



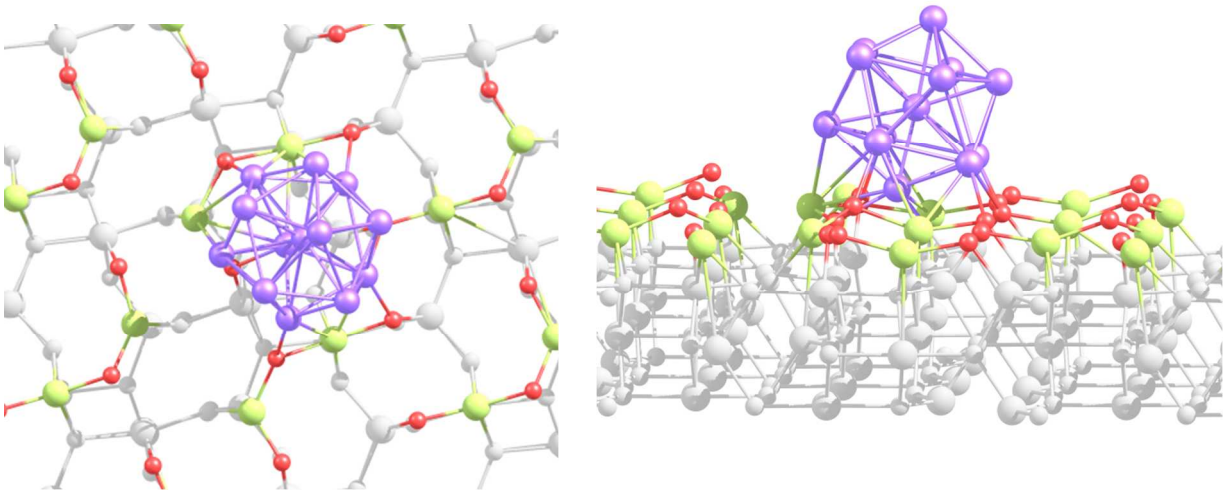
E_b= 7.25 eV

b)



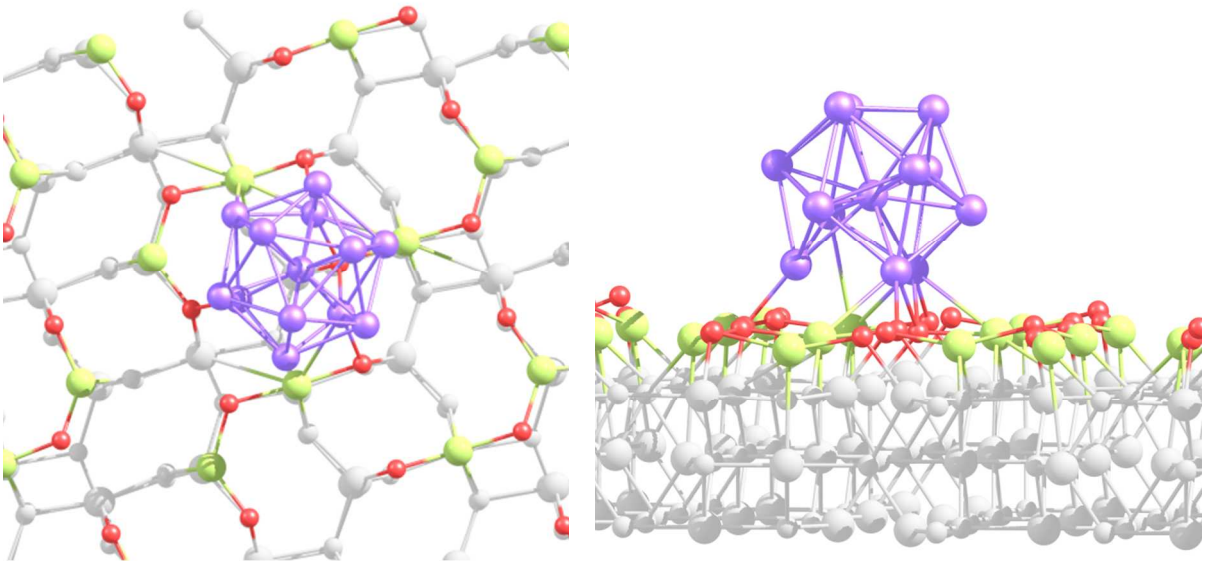
E_b= 5.69 eV

c)



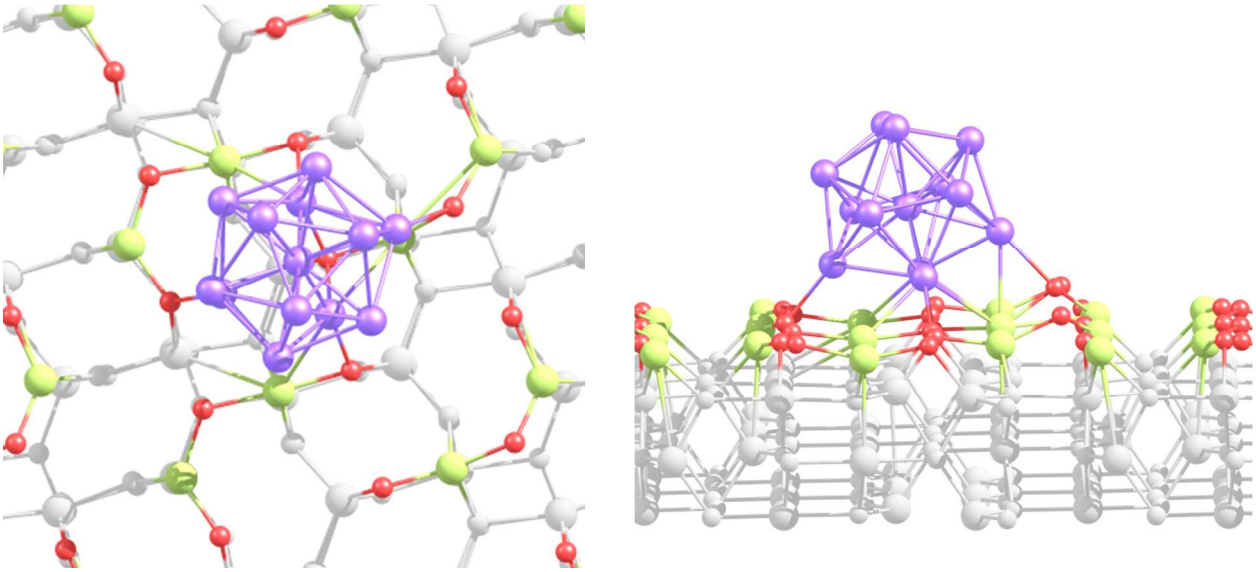
E_b= 5.48 eV

d)



E_b= 5.31 eV

e)



E_b= 5.21 eV

Figure S2. Optimized structures of ico-Ni_{13} cluster on θ-Al_2O_3(010) surface (a)-(e). Ni prefers maximize interaction with the low coordinated O atoms resulting in strong deformations of the cluster, especially noticeable in the most bounded (a) and (b) configurations. Aluminum atoms are yellow-green-colored and oxygen atoms are red-colored. Only the first layer atoms of the surface are colored, while the deeper layers are shown in light gray.

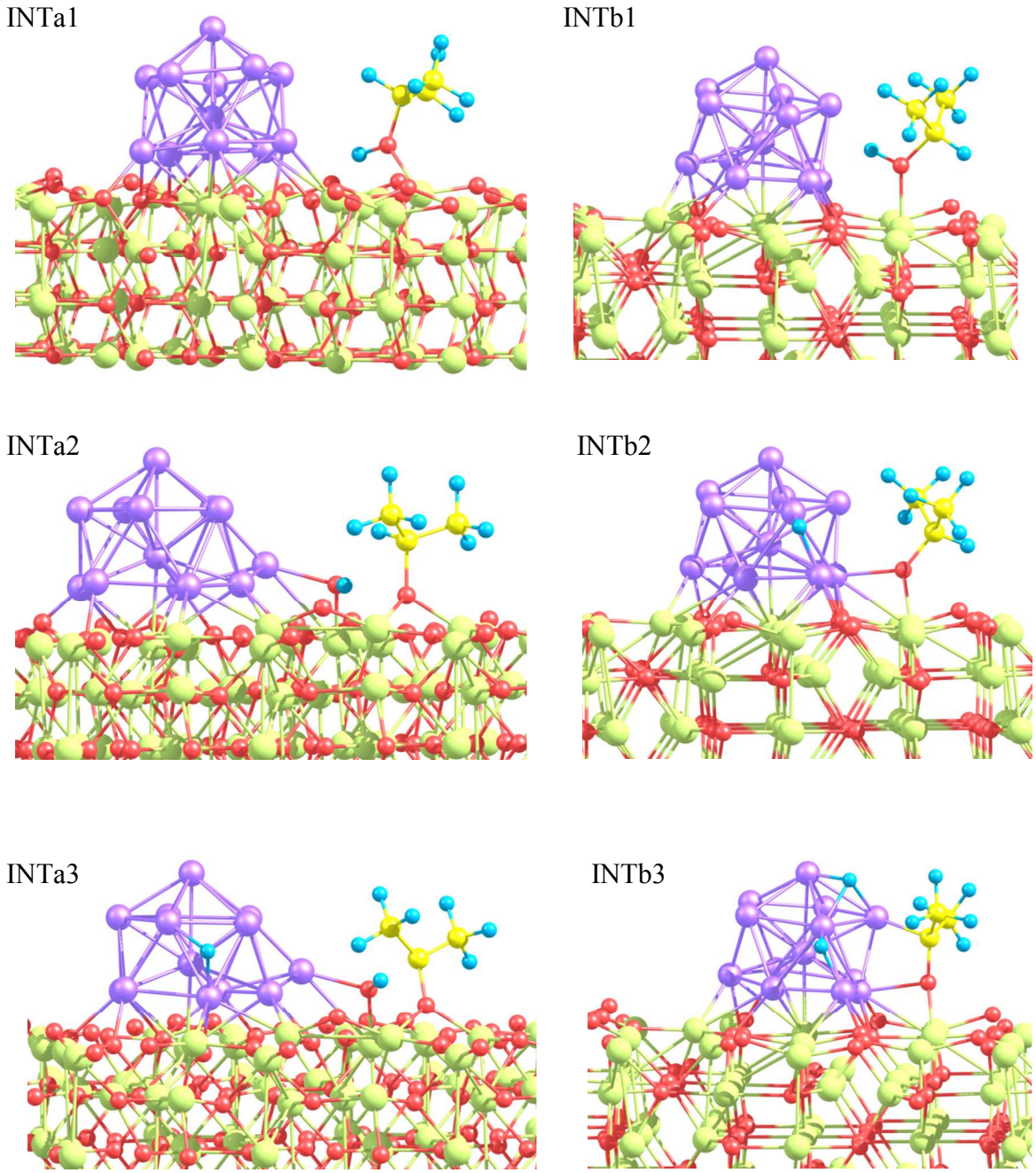


Figure S3. Optimized structures of C_3H_8O adsorbed on the θ-Al_2O_3(010) surface in the close vicinity of Ni_{13} cluster INTa1 and INTb1 (upper row); optimized structures of intermediates INTa2 and INTb2 formed after first H transfer from the OH group of isopropanol (middle row); optimized structures of intermediates INTa3 and INTb3 formed after C-H bond cleavage (lower row).