Electronic Supplementary Information

The Growth of Ni_n Clusters and Their Interaction with Cubic, Monoclinic, and Tetragonal ZrO_2 Surfaces–A Theoretical and Experimental Study

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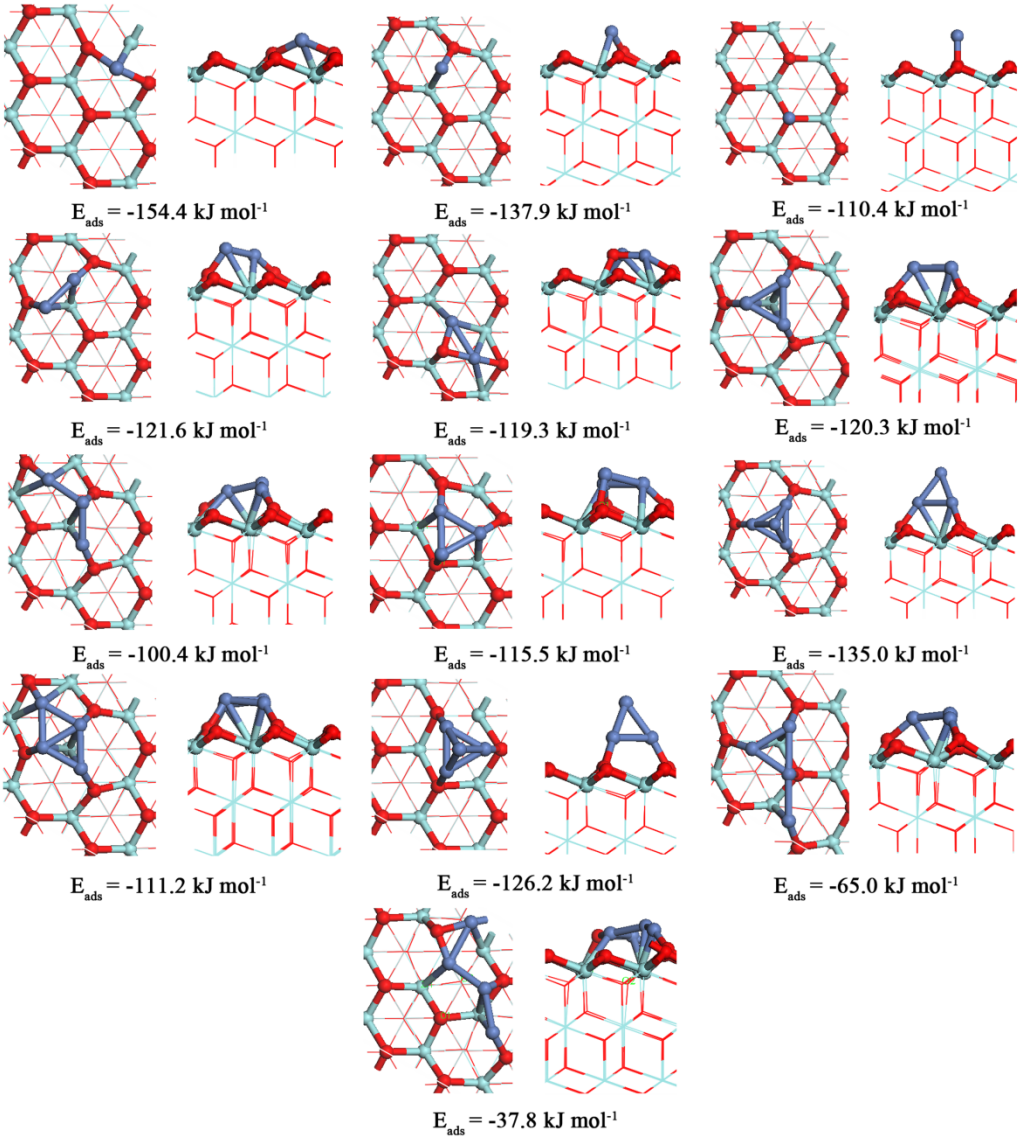
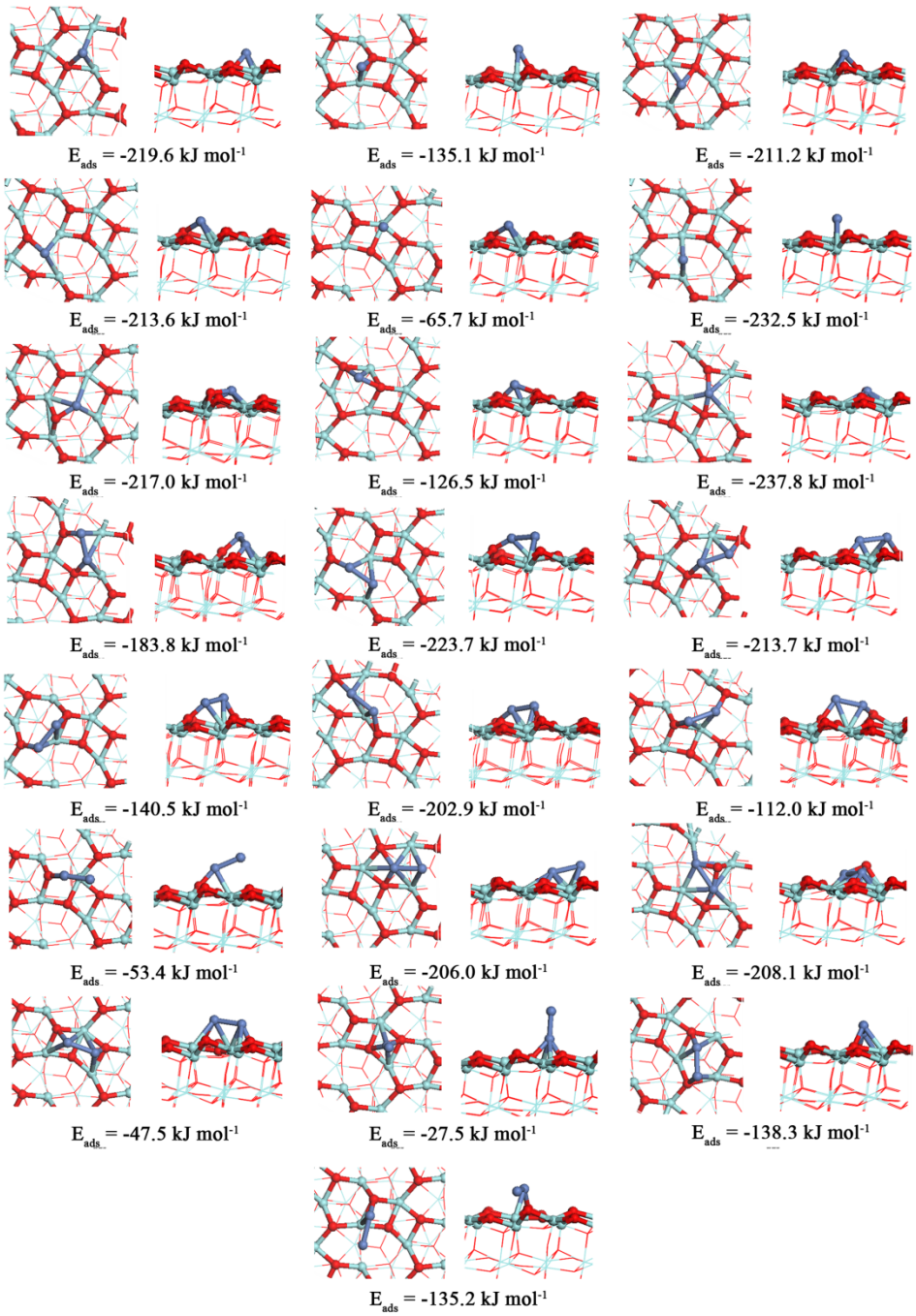


Figure S1. All the adsorption configurations and the corresponding energies of Ni_n (n = 1-4) structures adsorbed on the c-ZrO_2(111) surface at all possible sites.

(a)


E_{ads} = -219.6 kJ mol^{-1}
E_{ads} = -135.1 kJ mol^{-1}
E_{ads} = -211.2 kJ mol^{-1}
E_{ads} = -213.6 kJ mol^{-1}
E_{ads} = -65.7 kJ mol^{-1}
E_{ads} = -232.5 kJ mol^{-1}
E_{ads} = -217.0 kJ mol^{-1}
E_{ads} = -126.5 kJ mol^{-1}
E_{ads} = -237.8 kJ mol^{-1}
E_{ads} = -183.8 kJ mol^{-1}
E_{ads} = -223.7 kJ mol^{-1}
E_{ads} = -213.7 kJ mol^{-1}
E_{ads} = -140.5 kJ mol^{-1}
E_{ads} = -202.9 kJ mol^{-1}
E_{ads} = -112.0 kJ mol^{-1}
E_{ads} = -53.4 kJ mol^{-1}
E_{ads} = -206.0 kJ mol^{-1}
E_{ads} = -208.1 kJ mol^{-1}
E_{ads} = -47.5 kJ mol^{-1}
E_{ads} = -27.5 kJ mol^{-1}
E_{ads} = -138.3 kJ mol^{-1}
E_{ads} = -135.2 kJ mol^{-1}

(b)

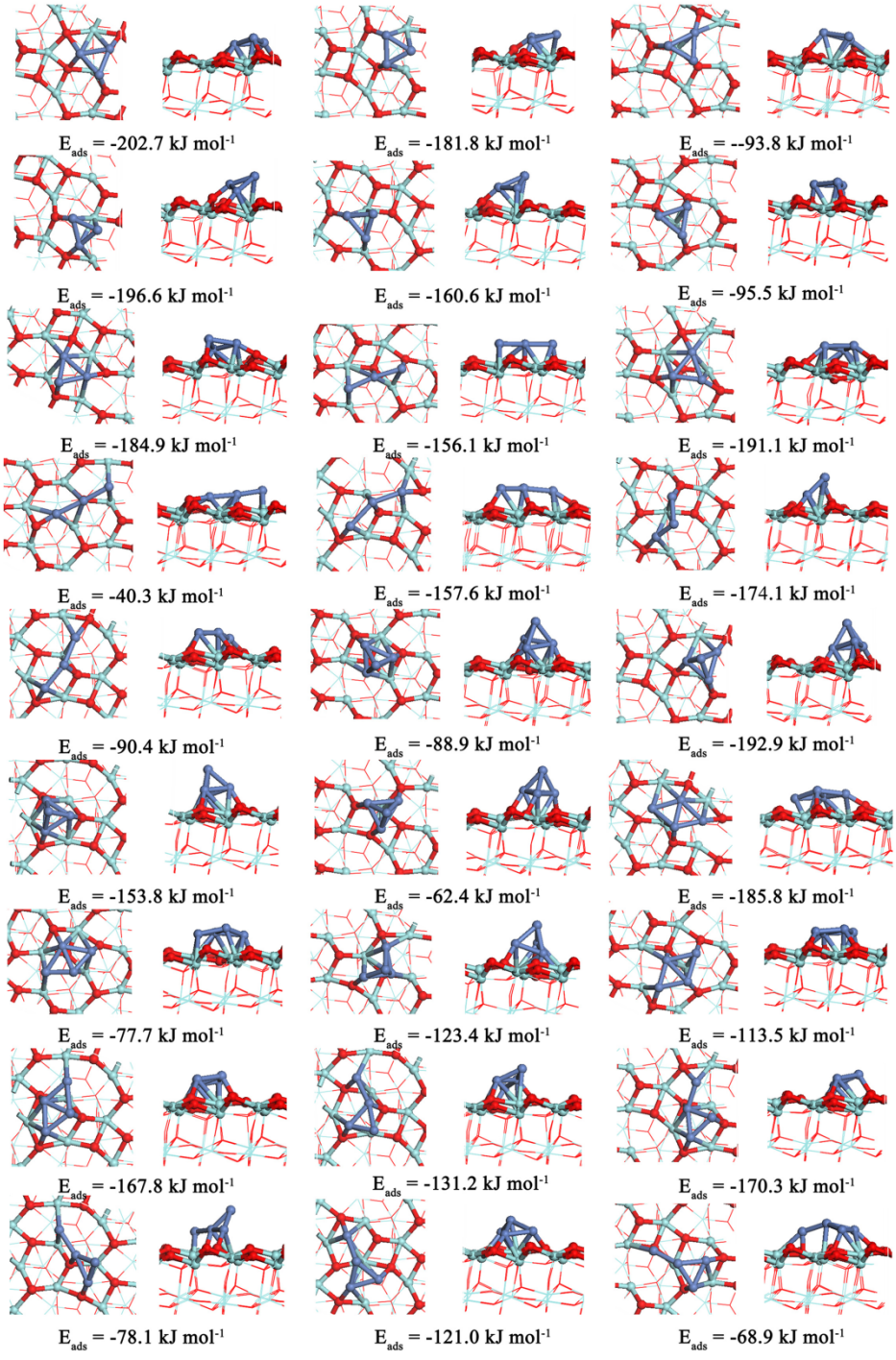
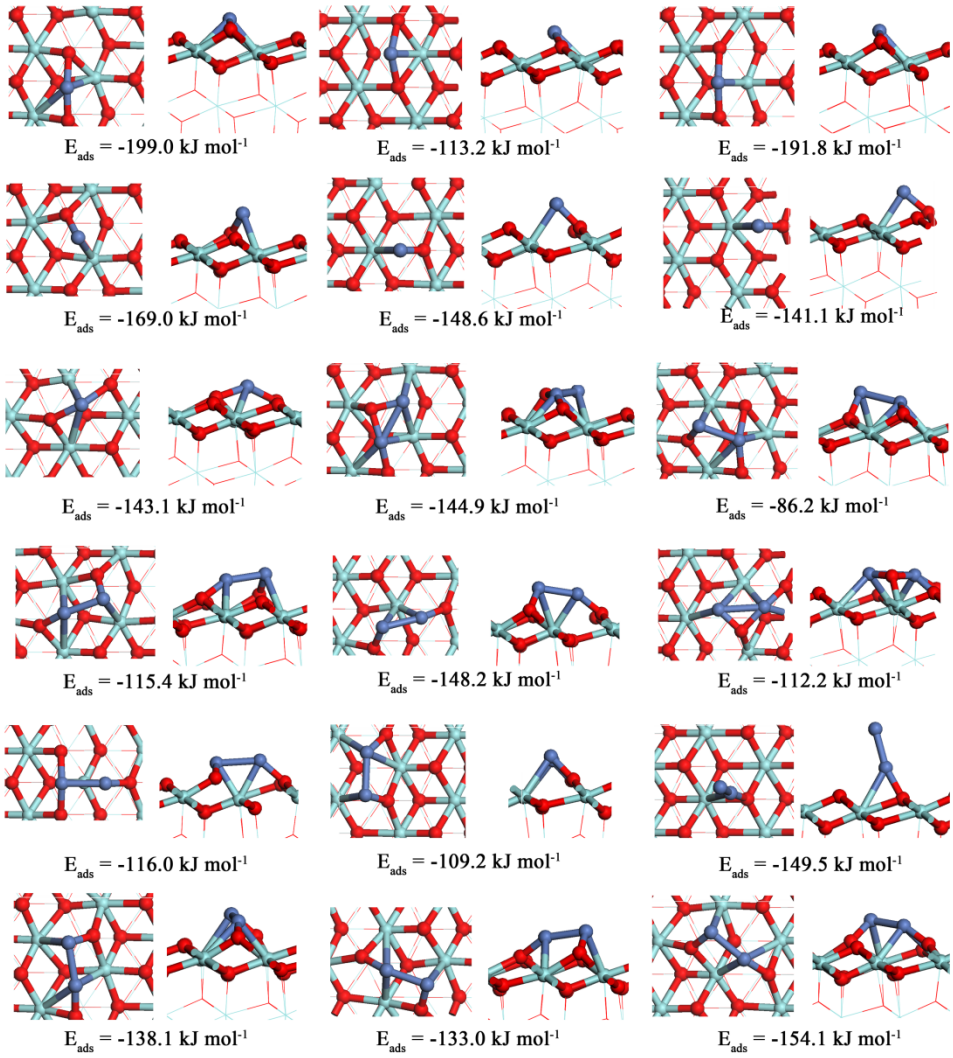


Figure S2. All the adsorption configurations and the corresponding energies of Ni_n (n = 1-4) structures adsorbed on the m-ZrO_2(111) surface at all possible sites.((a) for Ni_n (n = 1-2) and (b) for Ni_n (n = 3-4))

(a)


E_{ads} = -199.0 kJ mol^{-1}
E_{ads} = -113.2 kJ mol^{-1}
E_{ads} = -191.8 kJ mol^{-1}
E_{ads} = -169.0 kJ mol^{-1}
E_{ads} = -148.6 kJ mol^{-1}
E_{ads} = -141.1 kJ mol^{-1}
E_{ads} = -143.1 kJ mol^{-1}
E_{ads} = -144.9 kJ mol^{-1}
E_{ads} = -86.2 kJ mol^{-1}
E_{ads} = -115.4 kJ mol^{-1}
E_{ads} = -148.2 kJ mol^{-1}
E_{ads} = -112.2 kJ mol^{-1}
E_{ads} = -116.0 kJ mol^{-1}
E_{ads} = -109.2 kJ mol^{-1}
E_{ads} = -149.5 kJ mol^{-1}
E_{ads} = -138.1 kJ mol^{-1}
E_{ads} = -133.0 kJ mol^{-1}
E_{ads} = -154.1 kJ mol^{-1}

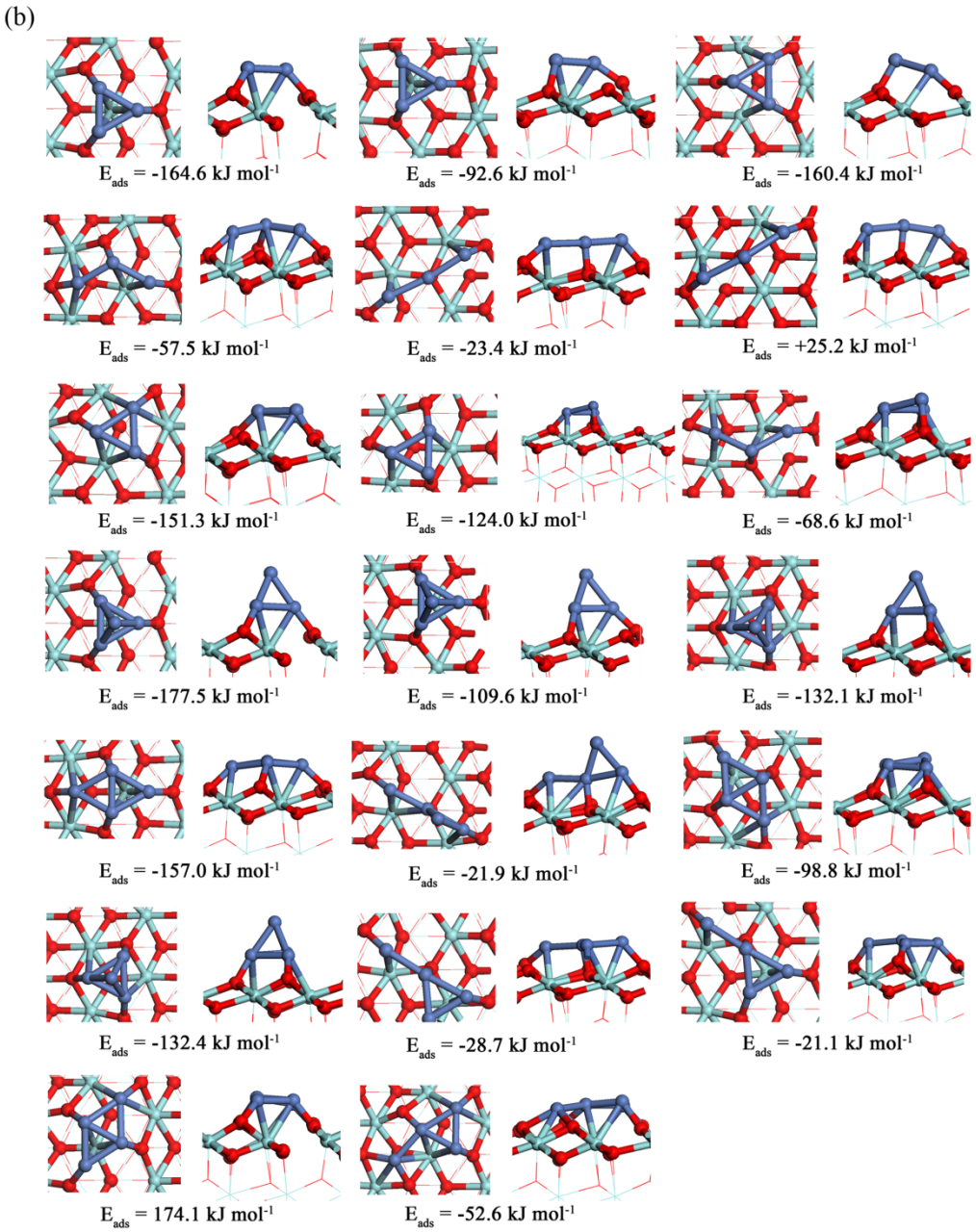


Figure S3. All the adsorption configurations and the corresponding energies of Ni_n (n = 1-4) structures adsorbed on the t-ZrO_2(111) surface at all possible sites.((a) for Ni_n (n = 1-2) and (b) for Ni_n (n = 3-4))