Stability and Mobility of Supported Ni_n (n = 1-10) Clusters on ZrO_2(111) and YSZ(111) Surfaces: a Density Functional Theory Study

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This document contains the less stable configurations and their respective binding energies of Ni clusters on ZrO_2(111) (**Figure S1** to **Figure S5**) and YSZ(111) (**Figure S6** to **Figure S21**) surfaces.

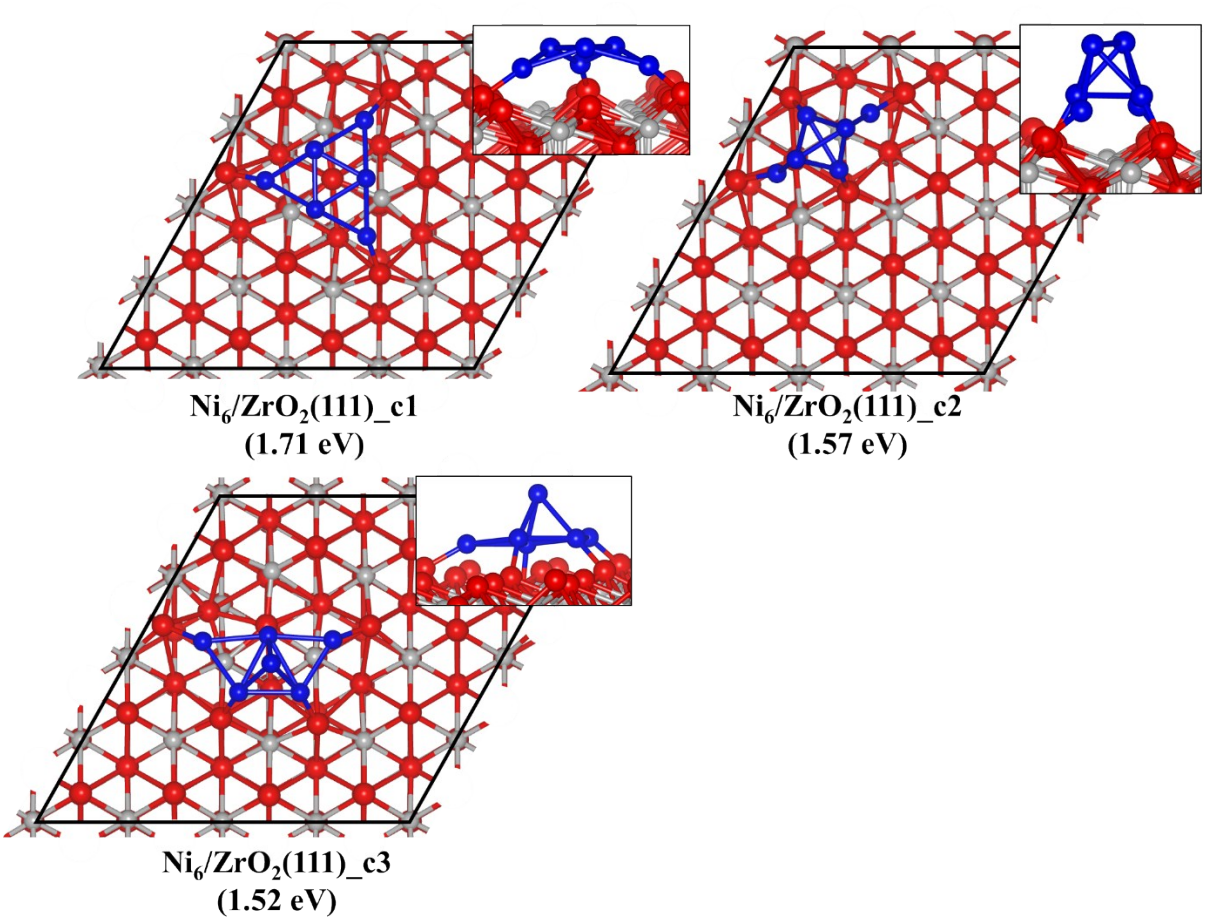

Figure S1. Top views (with side views as inset) of the less stable configurations of the $Ni_6/ZrO_2(111)$ system. The binding energies are in parenthesis. Colour key: red, grey, and blue spheres correspond to oxygen, Zr and Ni atoms, respectively.

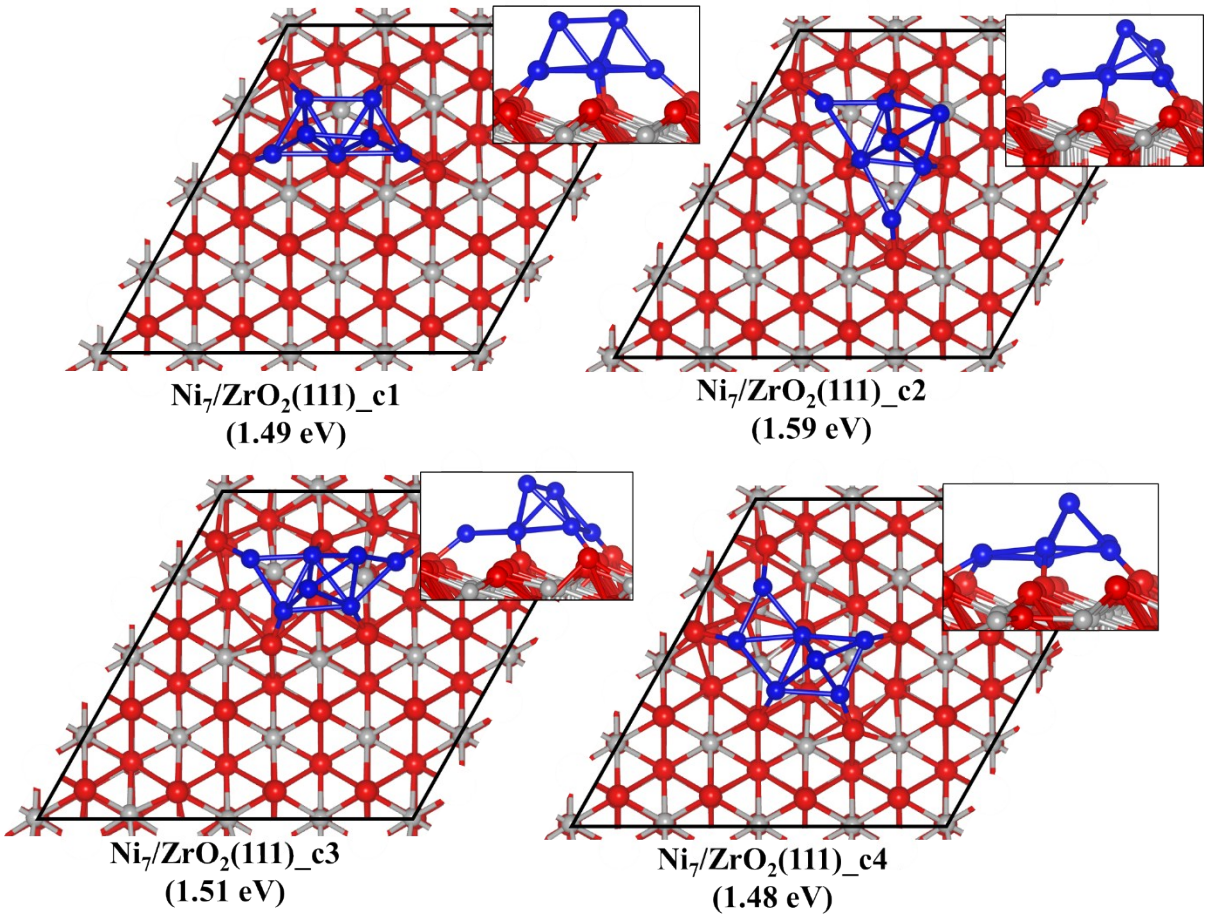

Figure S2. Top views (with side views as inset) of the less stable configurations of the $Ni_7/ZrO_2(111)$ system. The binding energies are in parenthesis. Colour key: red, grey, and blue spheres correspond to oxygen, Zr and Ni atoms, respectively.

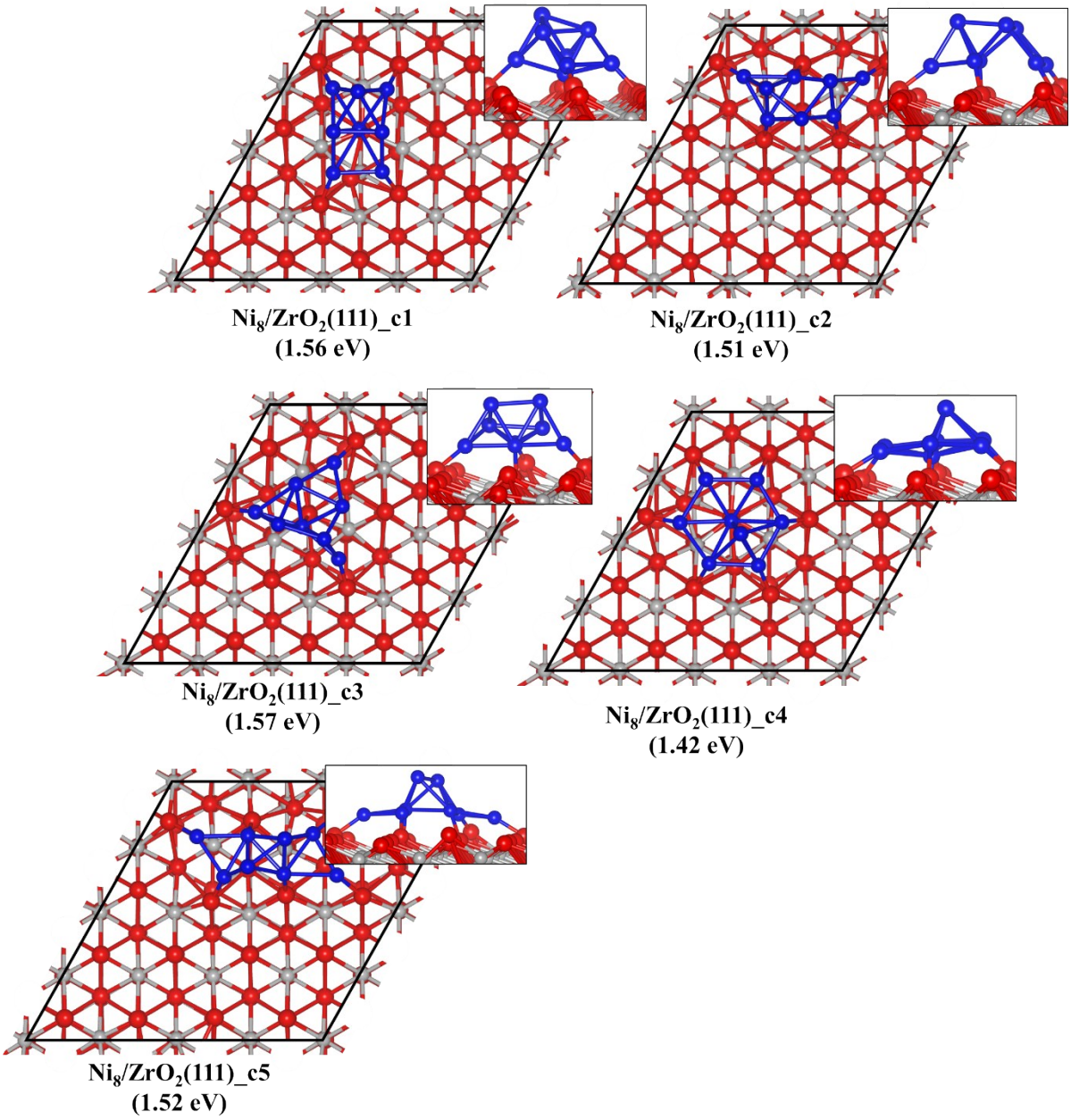

Figure S3. Top views (with side views as inset) of the less stable configurations of the $Ni_8/ZrO_2(111)$ system. The binding energies are in parenthesis. Colour key: red, grey, and blue spheres correspond to oxygen, Zr and Ni atoms, respectively.

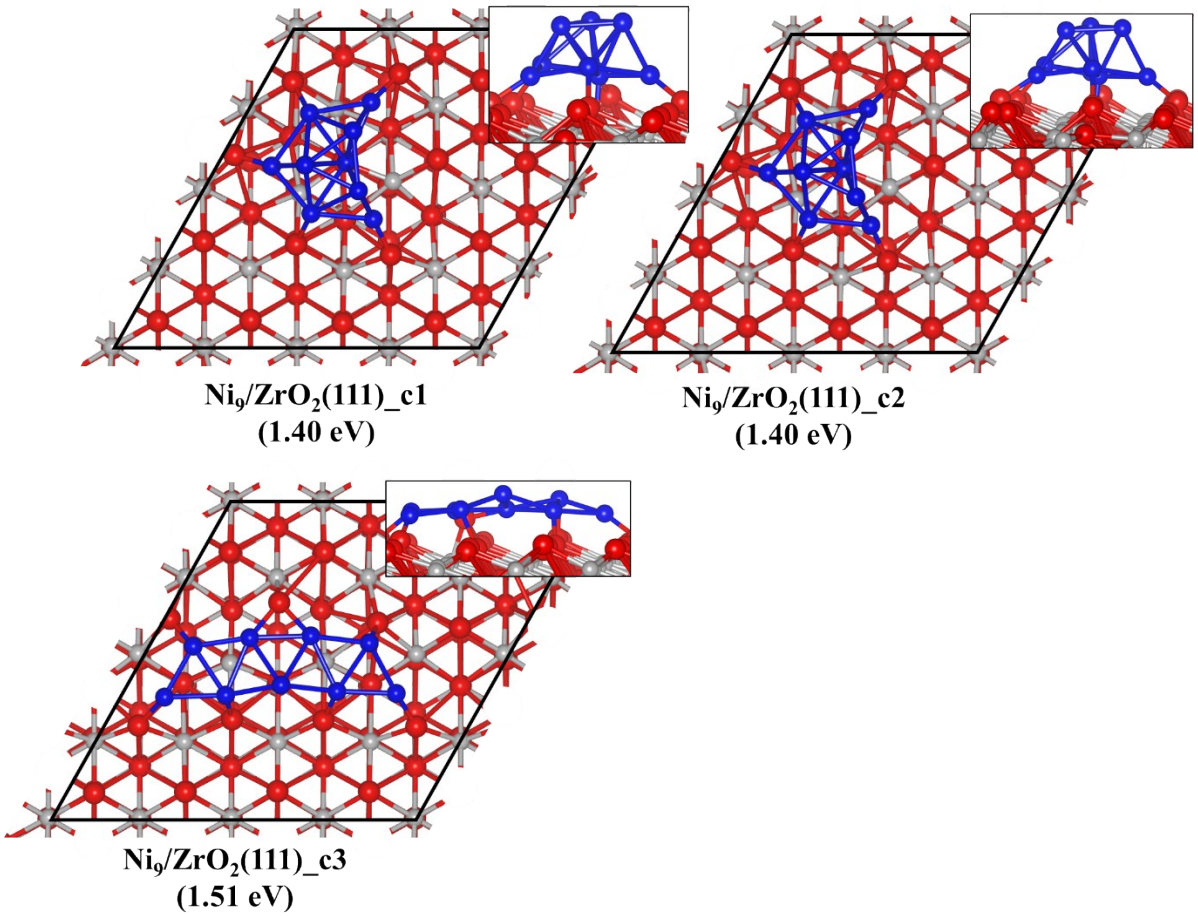

Figure S4. Top views (with side views as inset) of the less stable configurations of the $Ni_9/ZrO_2(111)$ system. The binding energies are in parenthesis. Colour key: red, grey, and blue spheres correspond to oxygen, Zr and Ni atoms, respectively.

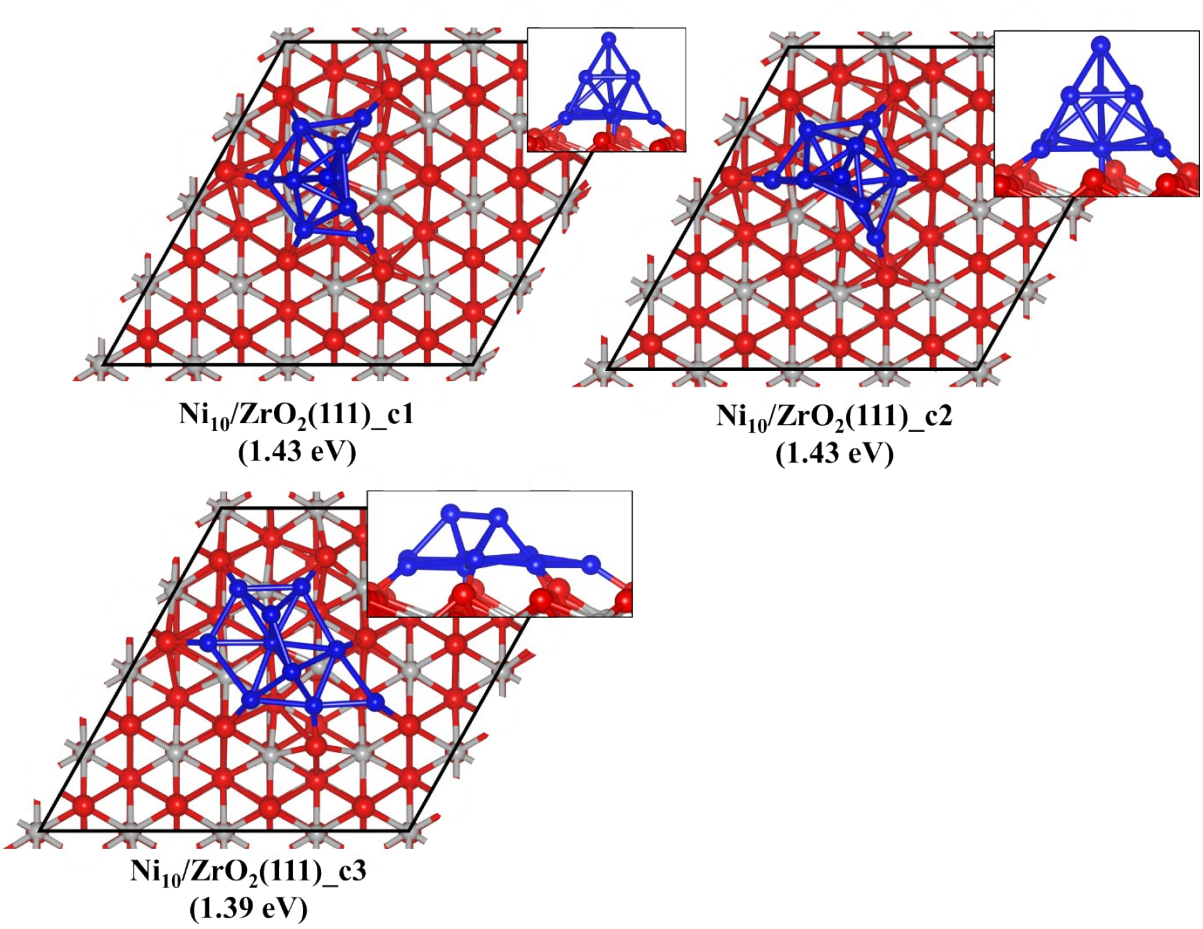

Figure S5. Top views (with side views as inset) of the less stable configurations of the $Ni_{10}/ZrO_2(111)$ system. The binding energies are in parenthesis. Colour key: red, grey, and blue spheres correspond to oxygen, Zr and Ni atoms, respectively.

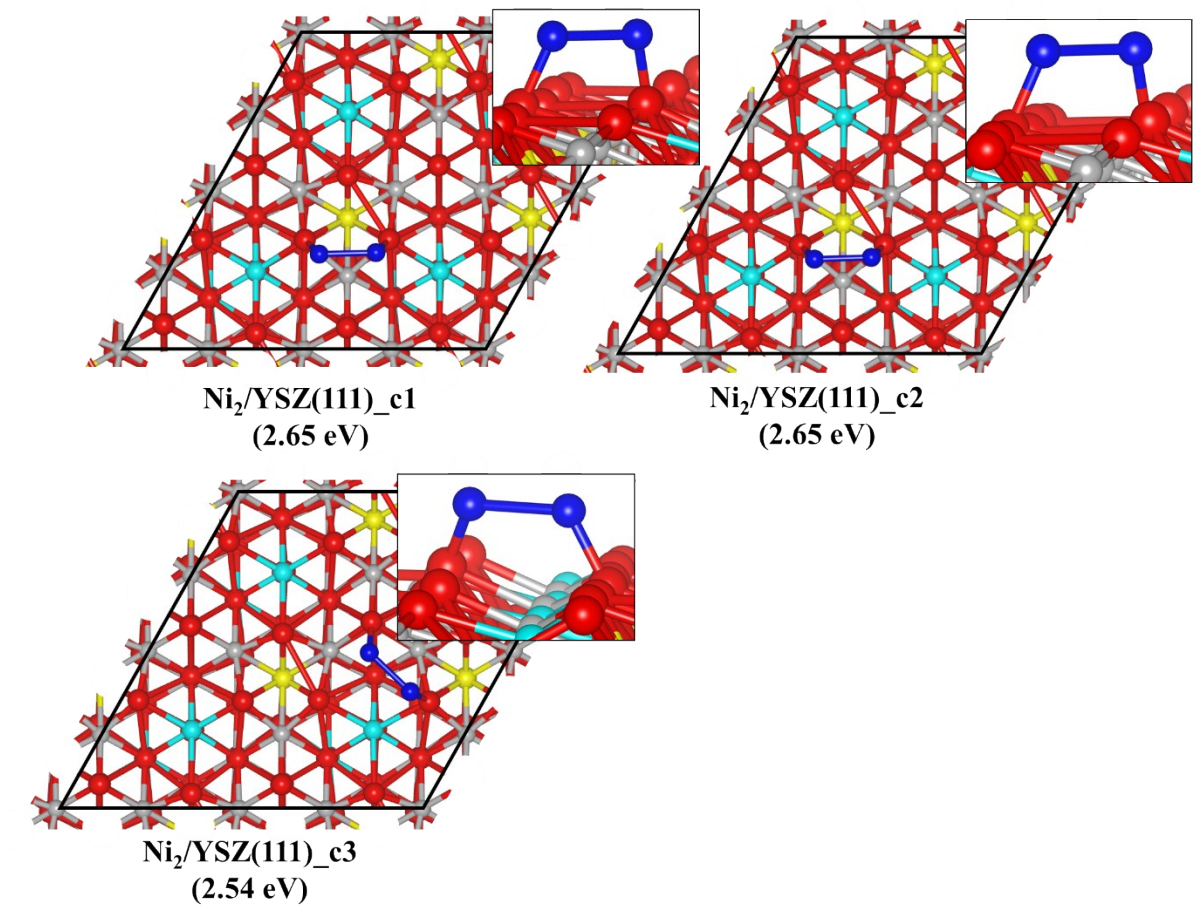

Figure S6. Top views (with side views as inset) of the less stable configurations of Ni_2/YSZ(111) systems. The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

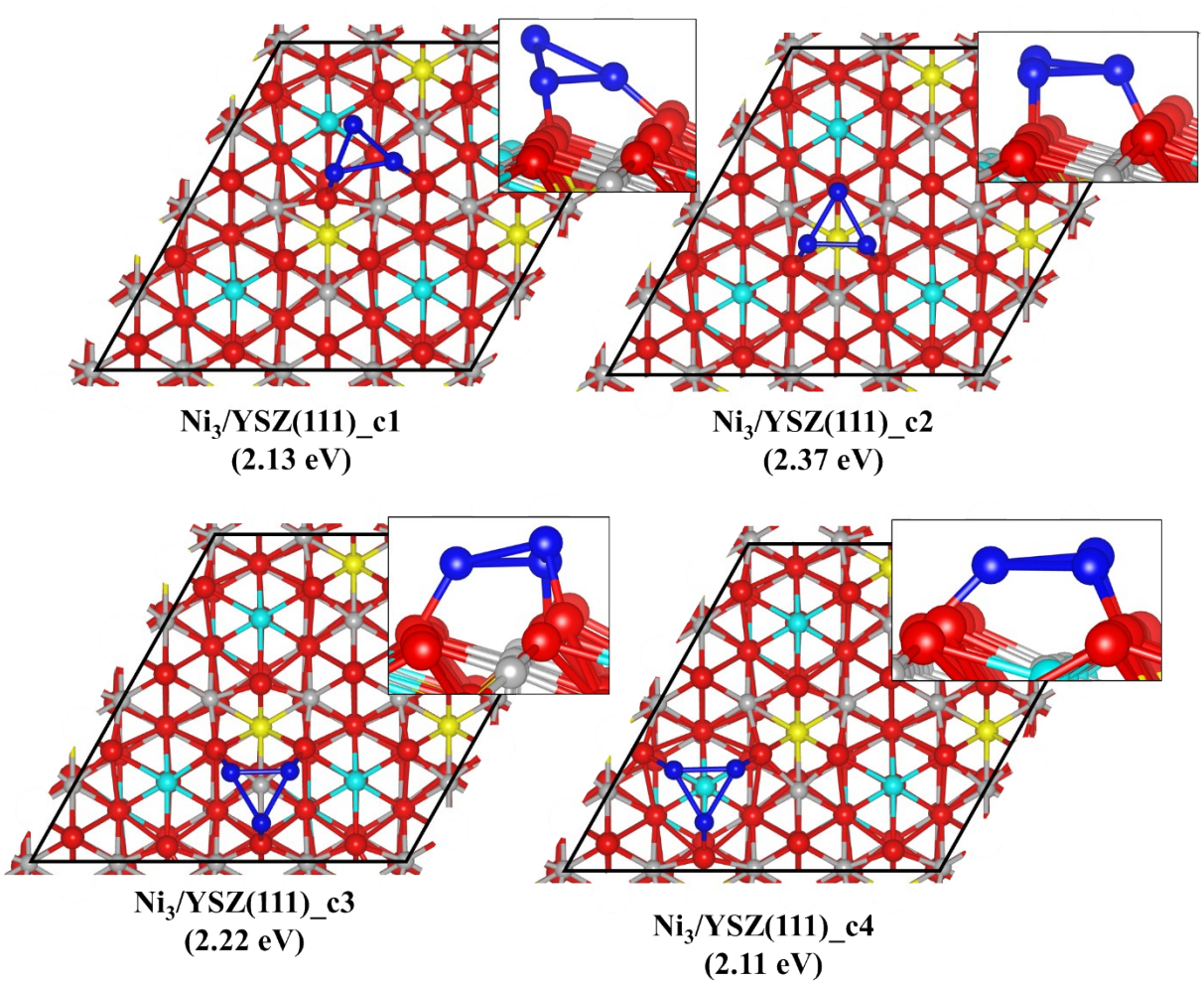

Figure S7. Top views (with side views as inset) of the less stable configurations of Ni_3/YSZ(111) systems. The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

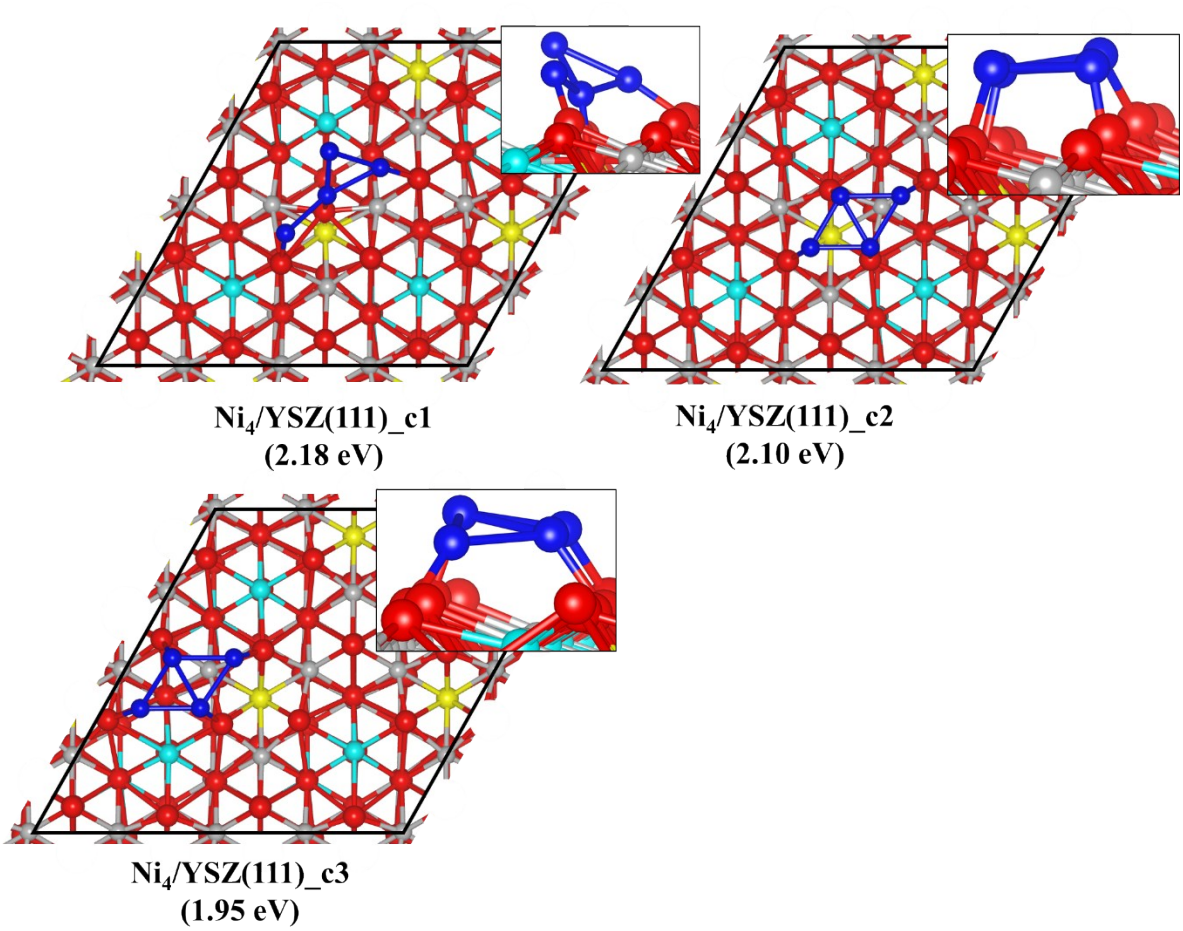

Figure S8. Top views (with side views as inset) of the less stable configurations of Ni_4/YSZ(111) systems (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

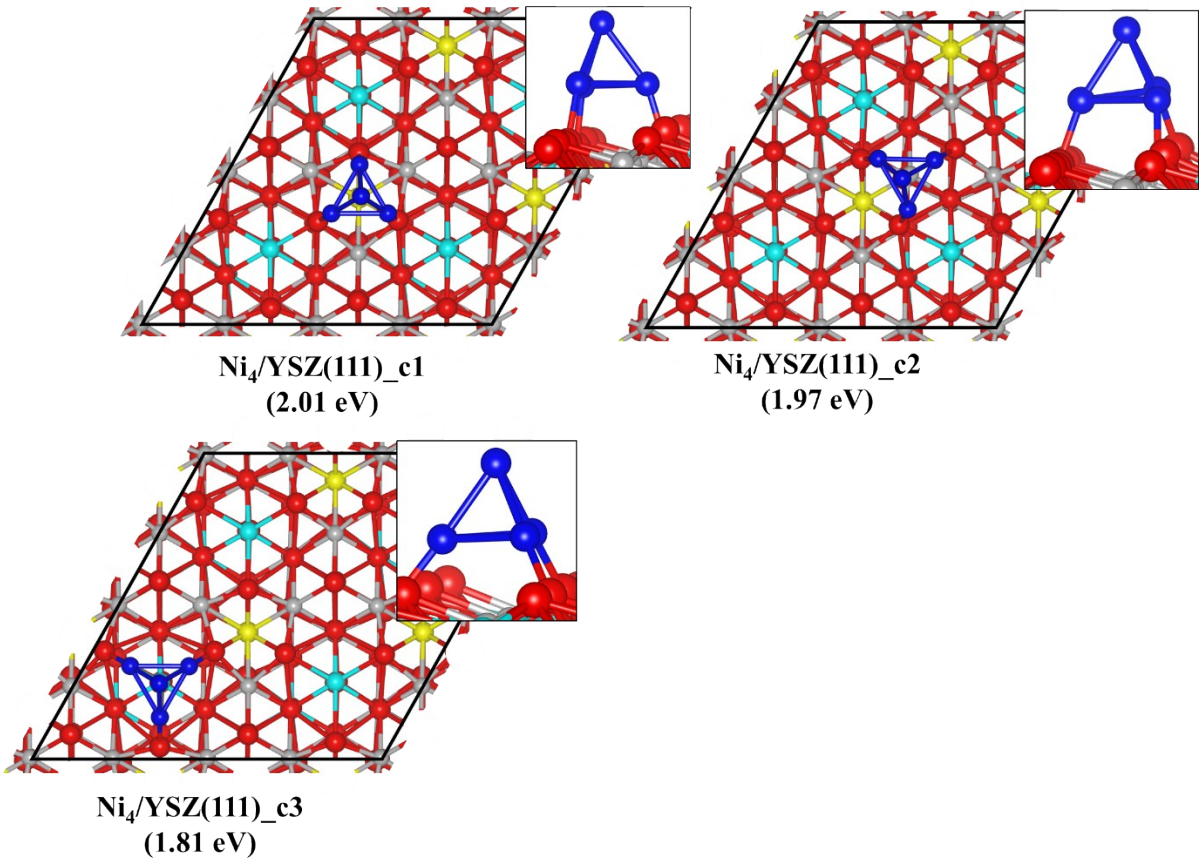

Figure S9. Top views (with side views as inset) of the less stable configurations of Ni_4/YSZ(111) systems (pyramid configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

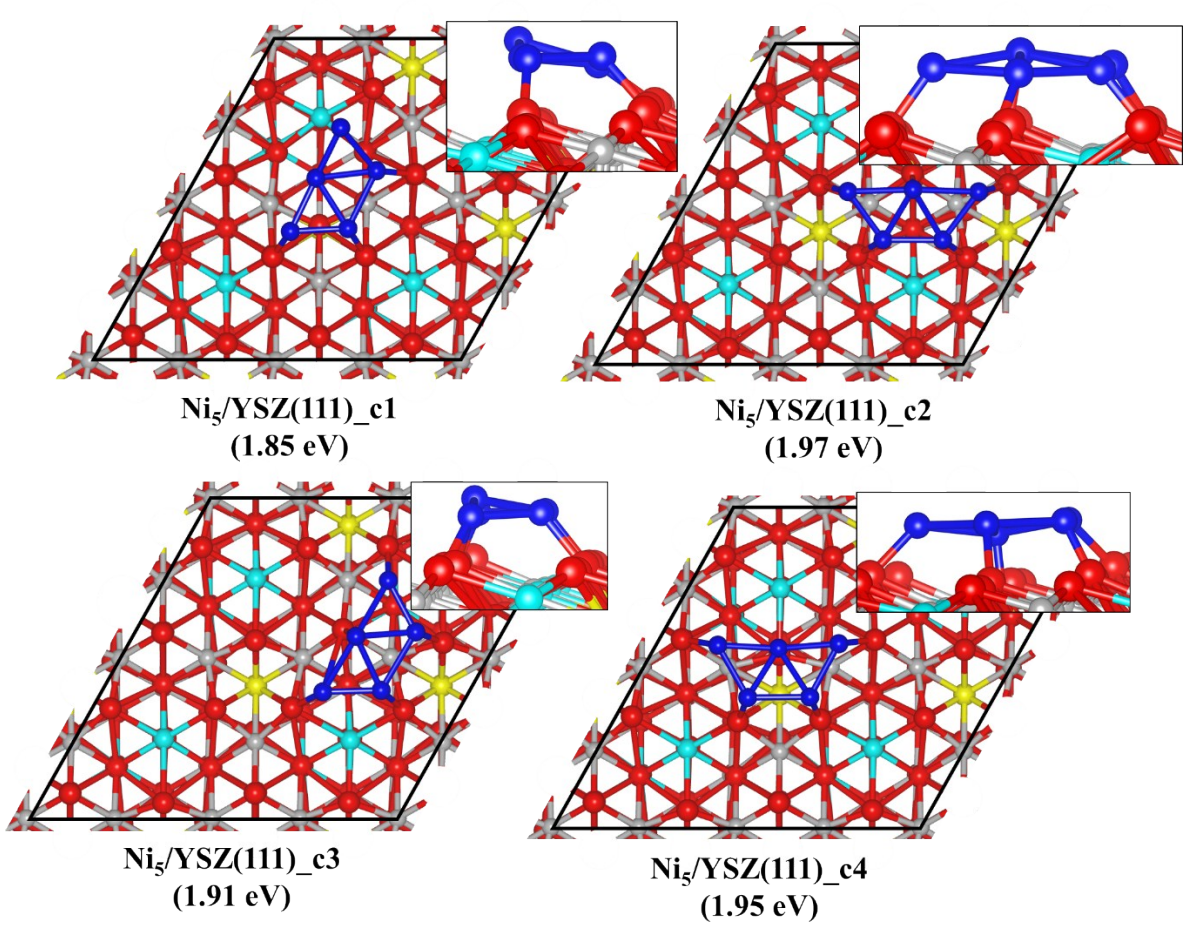

Figure S10. Top views (with side views as inset) of the less stable configurations of Ni_5/YSZ(111) systems (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

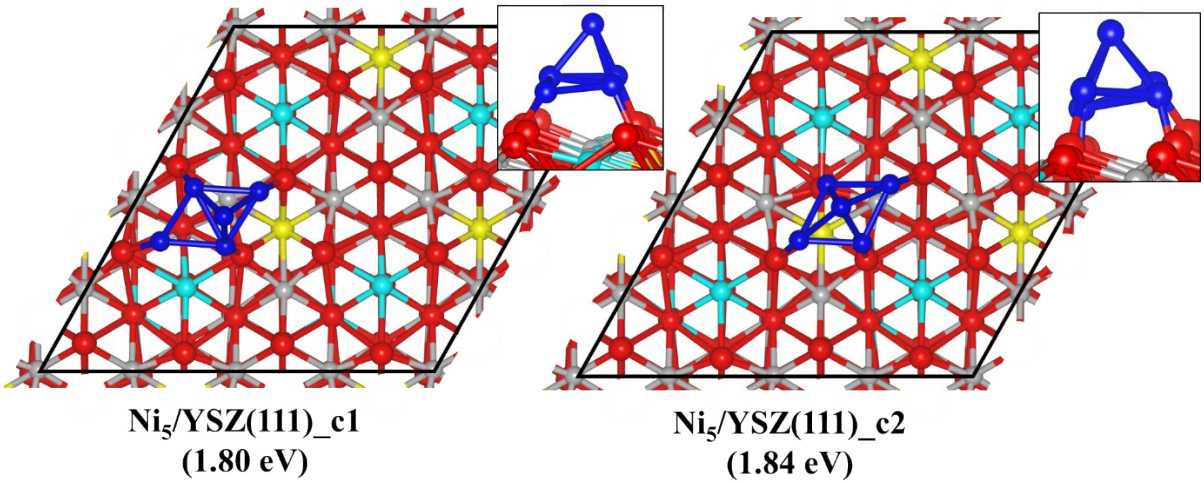

Figure S11. Top views (with side views as inset) of the non stable configurations of Ni_5/YSZ(111) systems (pyramid configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

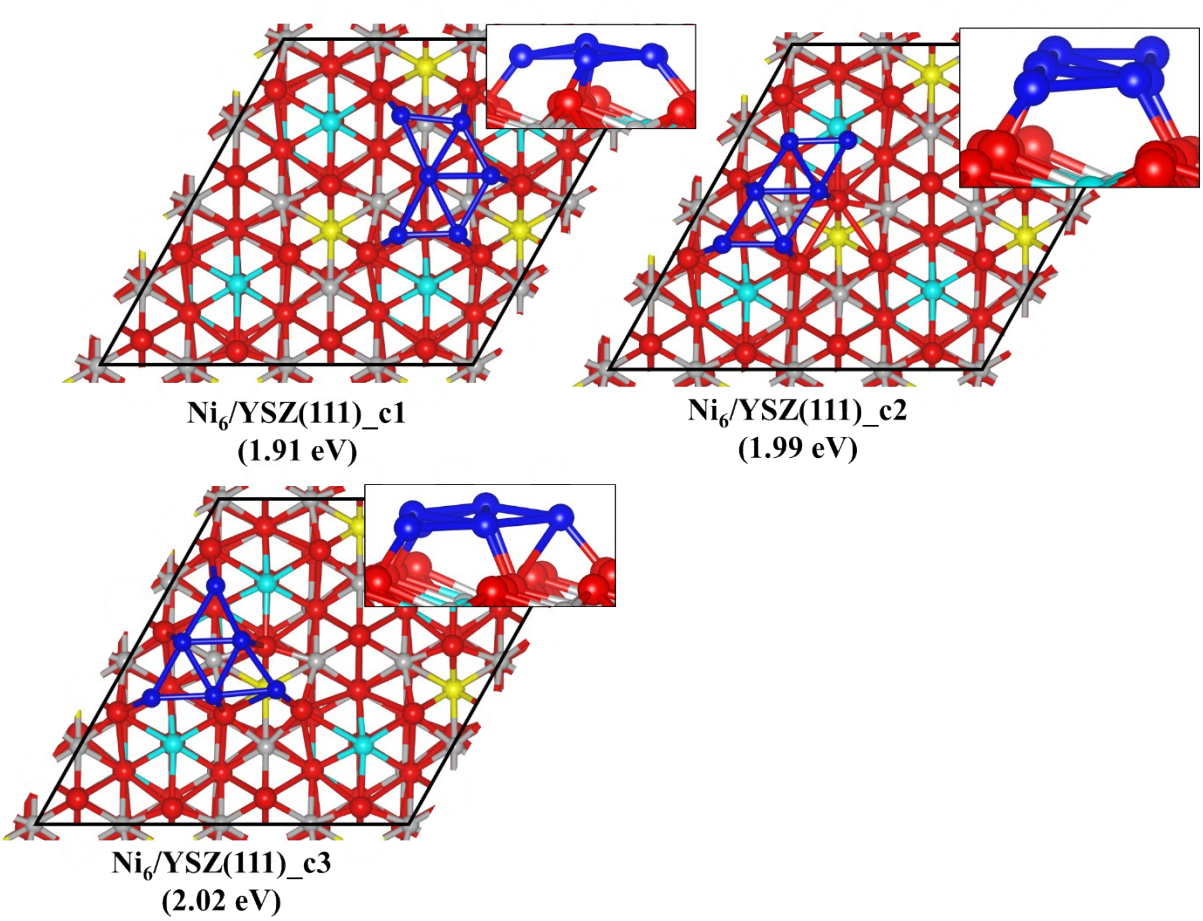

Figure S12. Top views (with side views as inset) of the less stable configurations of Ni_6/YSZ(111) systems (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

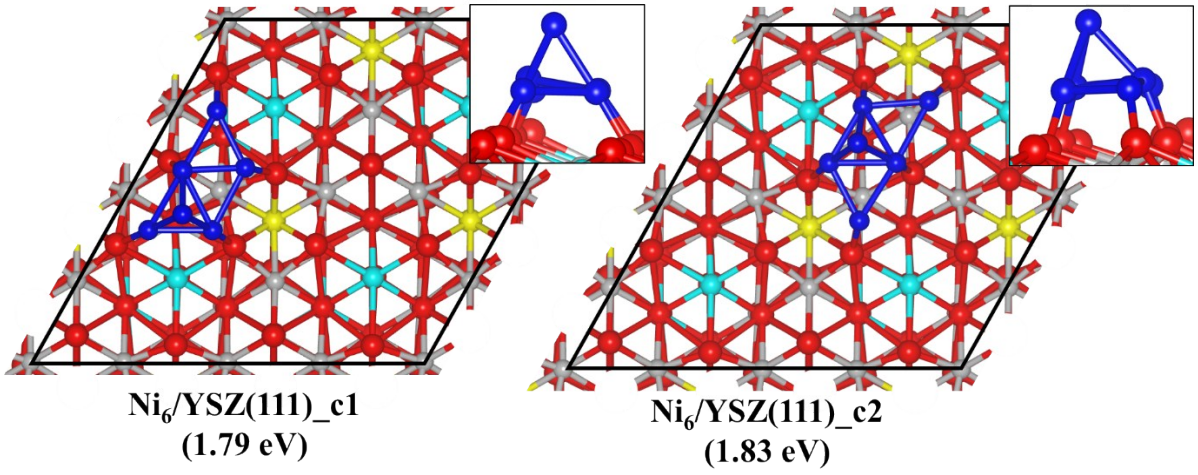

Figure S13. Top views (with side views as inset) of the less stable configurations of Ni_6/YSZ(111) systems (pyramid configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

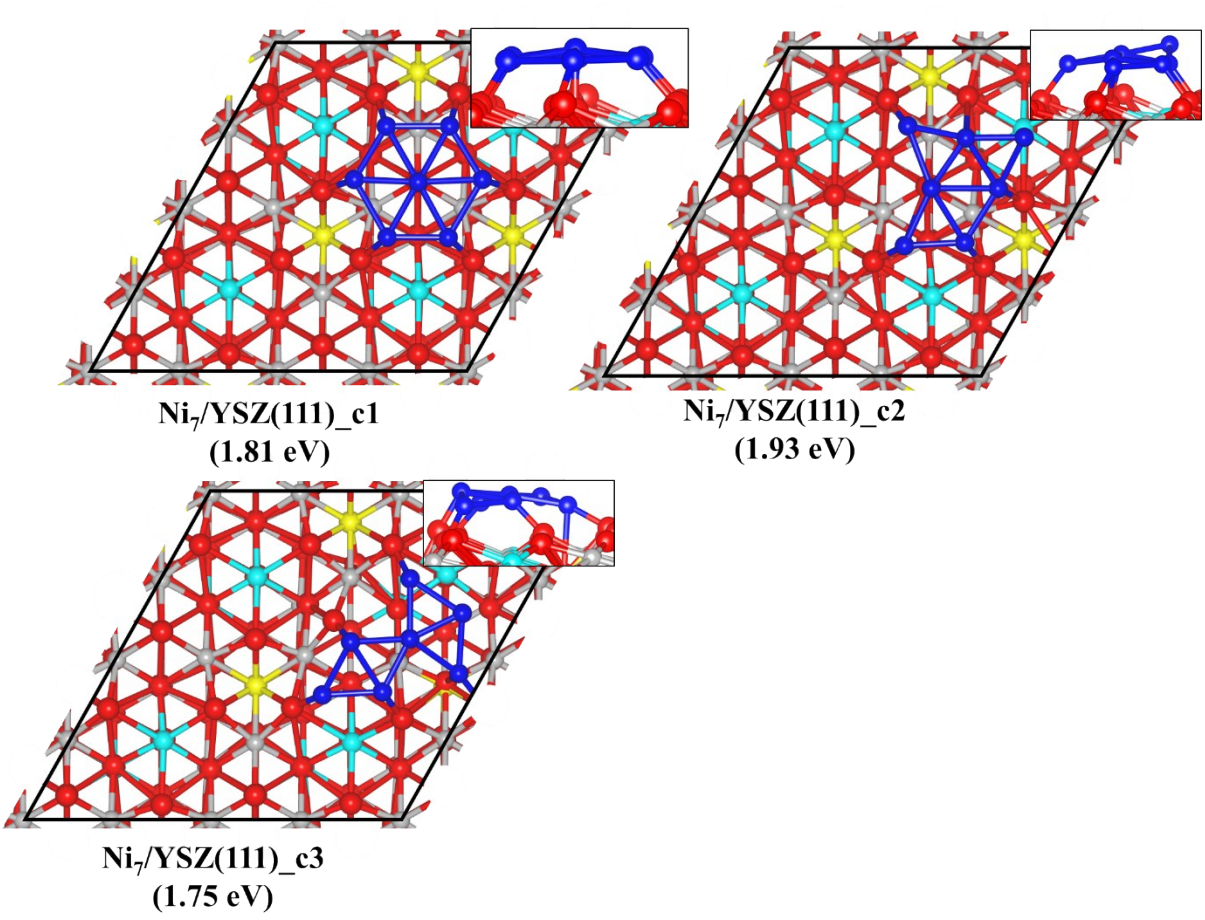

Figure S14. Top views (with side views as inset) of the less stable configurations of Ni_7/YSZ(111) systems (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

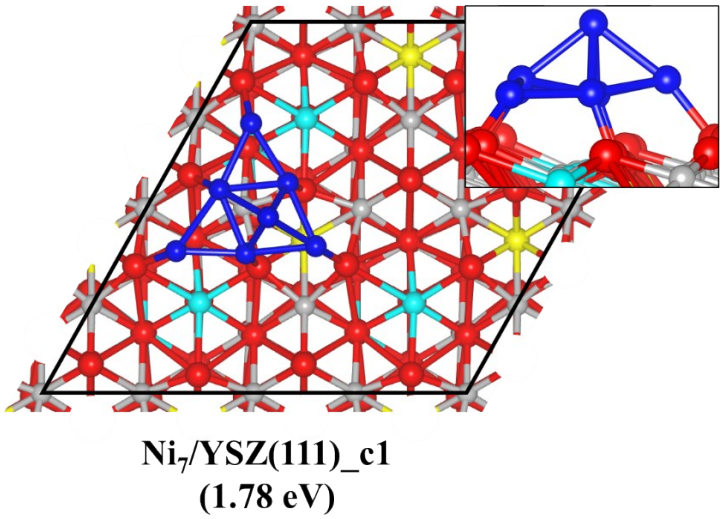

Figure S15. Top views (with side views as inset) of the less stable configuration of Ni_7/YSZ(111) system (pyramid configuration). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

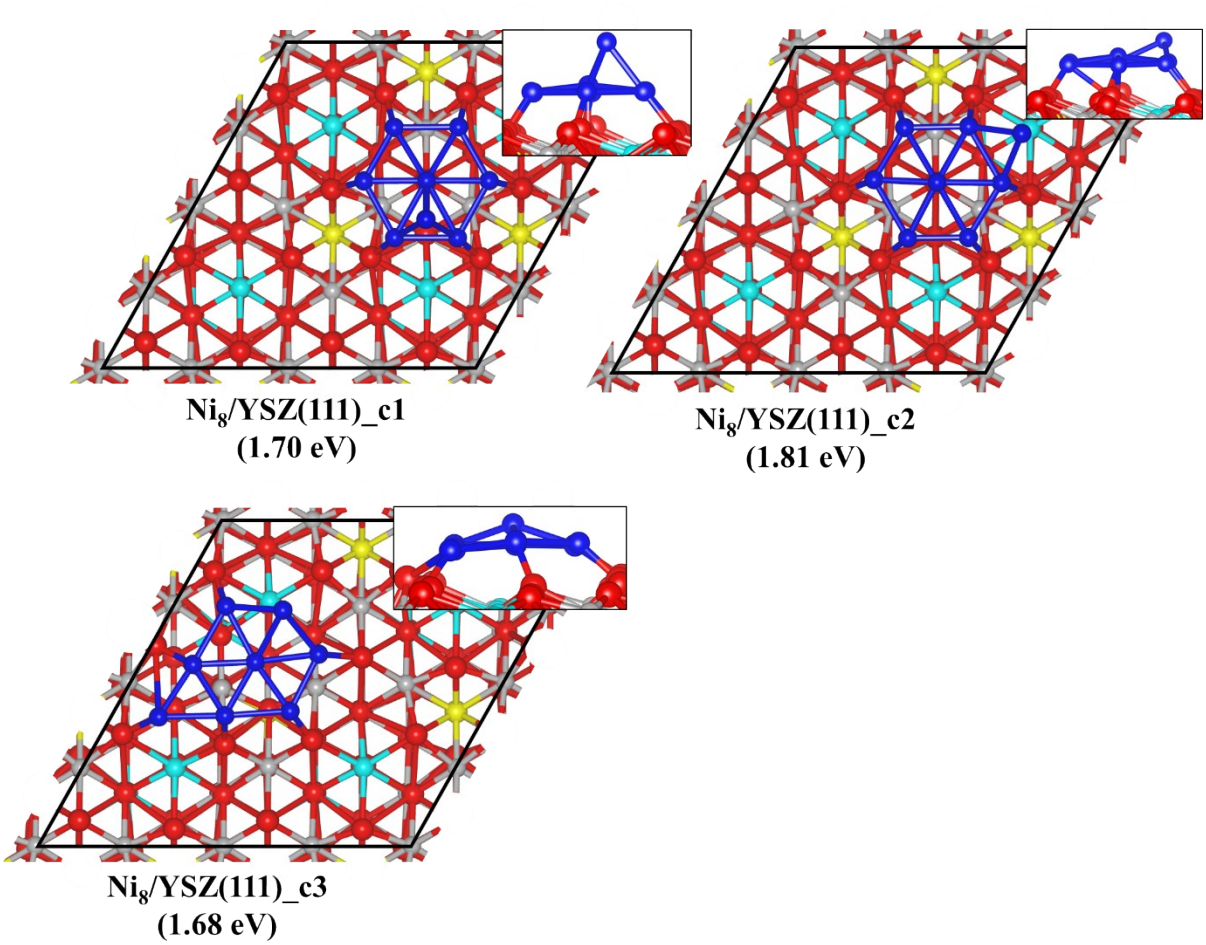

Figure S16. Top views (with side views as inset) of the less stable configurations of Ni_8/YSZ(111) systems (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

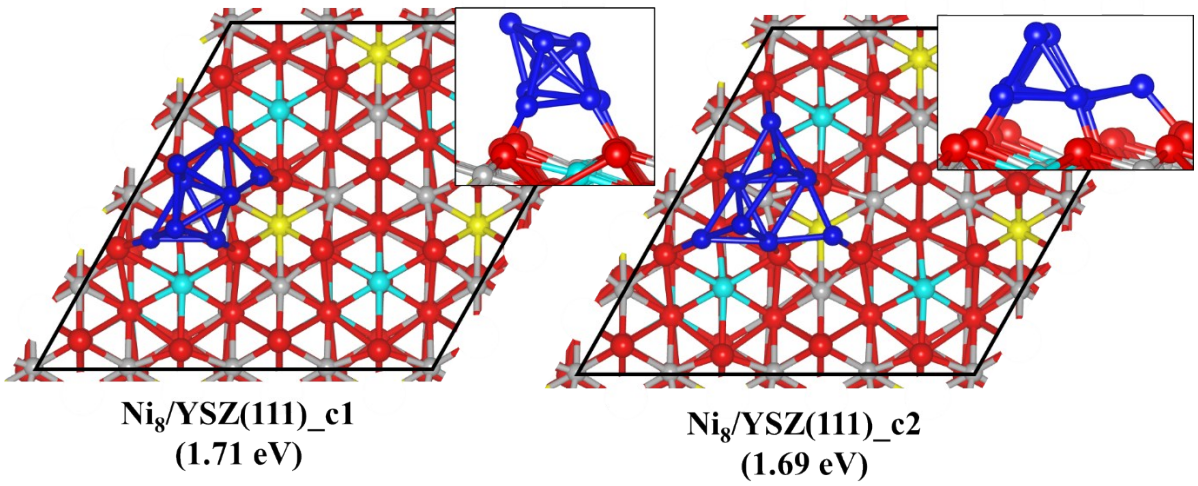

Figure S17. Top views (with side views as inset) of the less stable configurations of Ni_8/YSZ(111) systems (pyramid configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

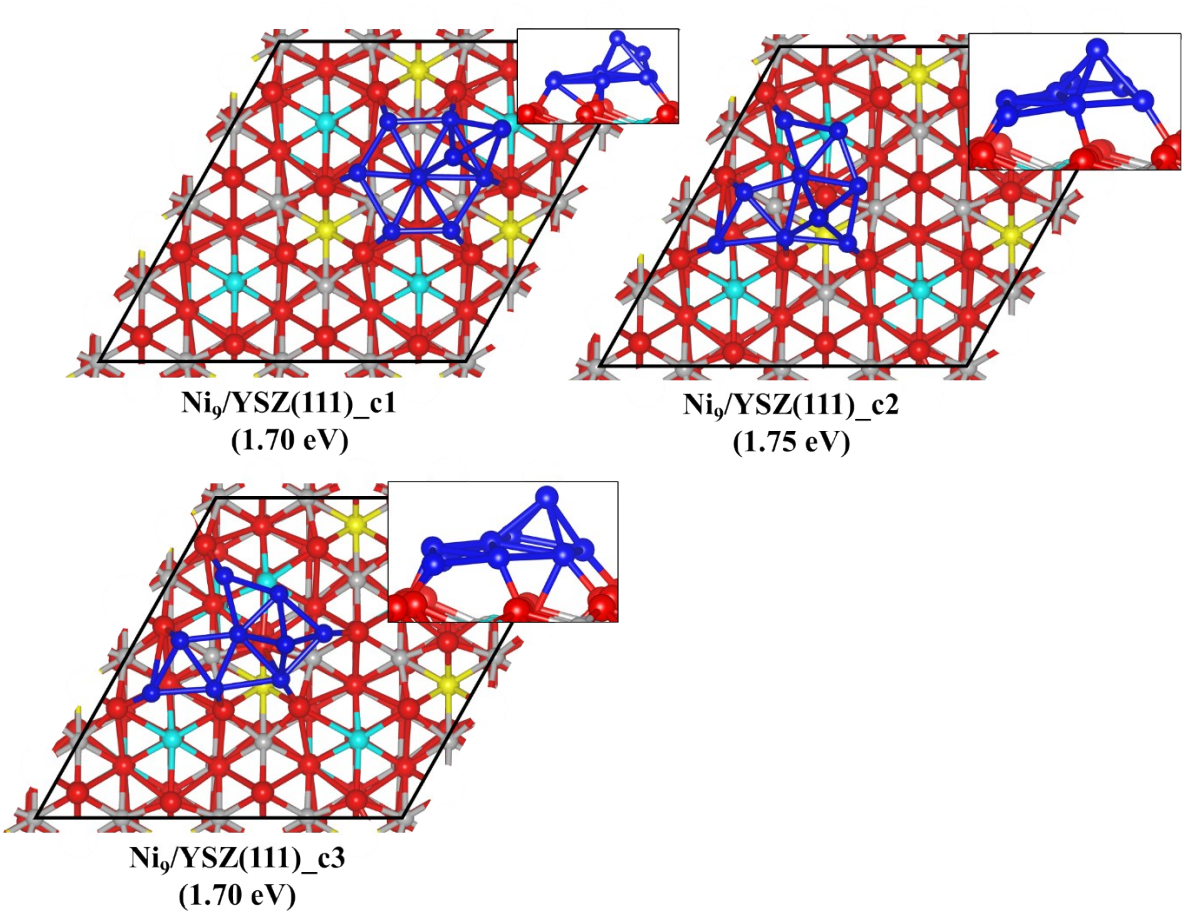

Figure S18. Top views (with side views as inset) of the less stable configurations of Ni_9/YSZ(111) systems (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

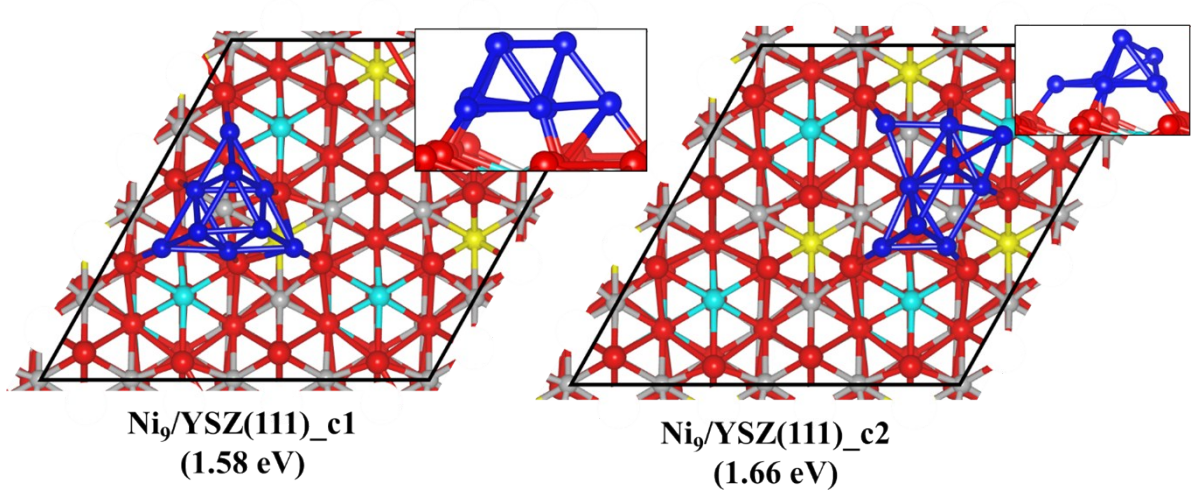

Figure S19. Top views (with side views as inset) of the less stable configurations of Ni_9/YSZ(111) systems (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

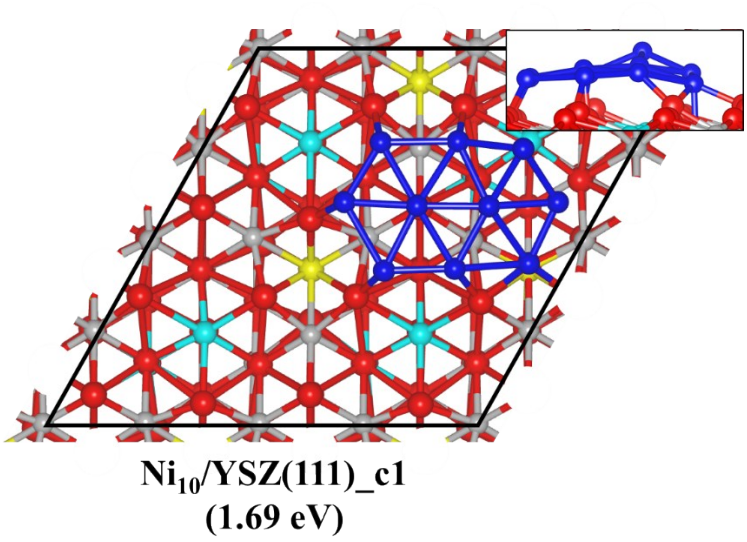

Figure S20. Top views (with side views as inset) of the less stable configuration of Ni_{10}/YSZ(111) system (flat configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.

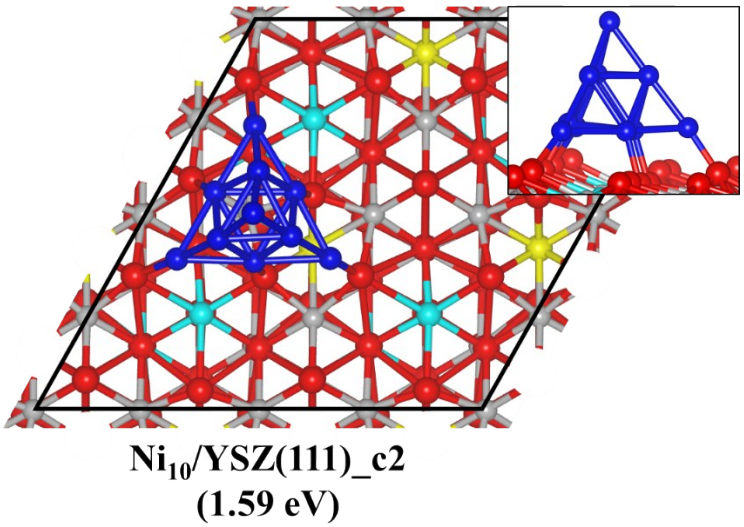

Figure S21. Top views (with side views as inset) of the less stable configuration of Ni_{10}/YSZ(111) system (pyramid configurations). The binding energies are in parenthesis. Colour key: red, grey, blue and cyan spheres correspond to oxygen, Zr, Ni and Y atoms, respectively. The oxygen vacancy is represented by a yellow sphere.