Supporting Information

Insight into Structure and Morphology of Ruₙ Clusters on Co(111) and Co(311) Surfaces

Lili Liuᵃᵇ, Mengting Yuᵃᵇ, Qiang Wangᵃ⁺*, Bo Houᵃ, Yan Liuᵃ, Yanbo Wuᶜ, Yongpeng Yangᵈ, and Debao Liᵃ⁺

ᵃ State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, Shanxi 030001, People’s Republic of China
ᵇ University of Chinese Academy of Sciences, Beijing 100049, People’s Republic of China
ᶜ The Key Lab of Materials for Energy Conversion and Storage of Shanxi Province, Institute of Molecular Science, Shanxi University, Taiyuan, People's Republic of China
ᵈ Research Center of Heterogeneous Catalysis and Engineering Sciences, School of Chemical Engineering and Energy, Zhengzhou University, Zhengzhou 450001, China

* Corresponding author at: No.27 Taoyuan Road, Taiyuan 030001, China. E-mail address: wqiang@sxicc.ac.cn (Qiang Wang) and dbli@sxicc.ac.cn (Debao Li)
Content

Figure S1. Various structures and adsorption energies for Ru\(_n\) (\(n = 1–2\)) on the Co(111) surface (adsorption energy in eV).

Figure S2. Various structures and adsorption energies for Ru\(_3\) on the Co(111) surface (adsorption energy in eV).

Figure S3. Various structures and adsorption energies for Ru\(_4\) on the Co(111) surface (adsorption energy in eV).

Figure S4. Various structures and adsorption energies for Ru\(_5\) on the Co(111) surface (adsorption energy in eV).

Figure S5. Various structures and adsorption energies for Ru\(_6\) on the Co(111) surface (adsorption energy in eV).

Figure S6. Various structures and adsorption energies for Ru\(_7\) on the Co(111) surface (adsorption energy in eV).

Figure S7. Various structures and adsorption energies for Ru\(_8\) on the Co(111) surface (adsorption energy in eV).

Figure S8. Various structures and adsorption energies for Ru\(_9\) on the Co(111) surface (adsorption energy in eV).

Figure S9. Various structures and adsorption energies for Ru\(_{10}\) on the Co(111) surface (adsorption energy in eV).

Figure S10. Various structures and adsorption energies for Ru\(_{11}\) on the Co(111) surface (adsorption energy in eV).

Figure S11. Various structures and adsorption energies for Ru\(_n\) (\(n = 1–3\)) on the Co(311) surface (adsorption energy in eV).

Figure S12. Various structures and adsorption energies for Ru\(_n\) (\(n = 4–5\)) on the Co(311) surface (adsorption energy in eV).

Figure S13. Various structures and adsorption energies for Ru\(_n\) (\(n = 6–8\)) on the Co(311) surface (adsorption energy in eV).

Figure S14. Various structures and adsorption energies for Ru\(_n\) (\(n = 11\)) on the Co(311) surface (adsorption energy in eV).

Figure S15. The average adsorption energy and growth energy variation with respect to the Ru cluster size on Co(111) and Co(311) surfaces.
Figure S1. Various structures and adsorption energies for Ru\textsubscript{n} (n = 1–2) on the Co(111) surface (adsorption energy in eV).
Figure S2. Various structures and adsorption energies for Ru$_3$ on the Co(111) surface (adsorption energy in eV).
Figure S3. Various structures and adsorption energies for Ru₄ on the Co(111) surface (adsorption energy in eV).
Figure S4. Various structures and adsorption energies for Ru$_5$ on the Co(111) surface (adsorption energy in eV).
Figure S5. Various structures and adsorption energies for Ru$_6$ on the Co(111) surface (adsorption energy in eV).
Figure S6. Various structures and adsorption energies for Ru$_7$ on the Co(111) surface (adsorption energy in eV).
Figure S7. Various structures and adsorption energies for Ru$_8$ on the Co(111) surface (adsorption energy in eV).
Figure S8. Various structures and adsorption energies for Ru$_9$ on the Co(111) surface (adsorption energy in eV).
Figure S9. Various structures and adsorption energies for Ru$_{10}$ on the Co(111) surface (adsorption energy in eV).
Figure S10. Various structures and adsorption energies for Ru$_{11}$ on the Co(111) surface (adsorption energy in eV).
Figure S11. Various structures and adsorption energies for Ru$_n$ (n = 1–3) on the Co(311) surface (adsorption energy in eV).
Figure S12. Various structures and adsorption energies for Ru$_n$ (n = 4–5) on the Co(311) surface (adsorption energy in eV).
Co(311)-Ru₆-4×4

1(-35.97)  2(-35.59)  3(-35.58)  4(-35.51)  5(-35.44)

Co(311)-Ru₇-4×4

6(-35.39)  7(-35.06)  8(-35.00)  9(-34.98)

Co(311)-Ru₈-4×4

1(-42.05)  2(-41.74)  3(-41.66)  4(-41.65)

5(-41.64)  6(-41.26)  7(-41.20)

Figure S13. Various structures and adsorption energies for Ruₙ (n = 6–8) on the Co(311) surface (adsorption energy in eV).
Figure S14. Various structures and adsorption energies for Ru11 on the Co(311) surface (adsorption energy in eV).

Figure S15. The average adsorption energy and growth energy variation with respect to the Ru cluster size on Co(111) and Co(311) surfaces.