Electronic Supplementary Material (ESI) for Catalysis Science & Technology. This journal is © The Royal Society of Chemistry 2018

#### **Supporting Information**

#### Insight into Structure and Morphology of Ru<sub>n</sub> Clusters on Co(111) and Co(311) Surfaces

Lili Liu<sup>a,b</sup>, Mengting Yu<sup>a,b</sup>, Qiang Wang<sup>a,\*</sup>, Bo Hou<sup>a</sup>, Yan Liu<sup>a</sup>, Yanbo Wu<sup>c</sup>, Yongpeng Yang<sup>d</sup>, and

Debao Li<sup>a,\*</sup>

<sup>a</sup> State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, Shanxi 030001, People's Republic of China

<sup>b</sup> 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

<sup>\*</sup> Corresponding author at: No.27 Taoyuan Road, Taiyuan 030001, China. E-mail address: wqiang@sxicc.ac.cn (Qiang Wang) and <u>dbli@sxicc.ac.cn</u> (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<sub>9</sub> 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.

## Co(111)- $Ru_1$ -4×4



Co(111)-Ru<sub>2</sub>-4×4



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

# Co(111)-Ru<sub>3</sub>-4×4



Figure S2. Various structures and adsorption energies for  $Ru_3$  on the Co(111) surface (adsorption energy in eV).

### Co(111)-Ru<sub>4</sub>-4×4



 6(-20.82)
 7(-20.76)
 8(-20.72)
 9(-20.70)
 10(-20.65)





Figure S3. Various structures and adsorption energies for  $Ru_4$  on the Co(111) surface (adsorption energy in eV).

### Co(111)-Ru<sub>5</sub>-4×4



16(-26.13)

Figure S4. Various structures and adsorption energies for  $Ru_5$  on the Co(111) surface (adsorption energy in eV).

### Co(111)-Ru<sub>6</sub>-4×4



8(-32.90)

6(-32.94)

7(-32.90)

9(-32.90)

10(-32.79)

Figure S5. Various structures and adsorption energies for  $Ru_6$  on the Co(111) surface (adsorption energy in eV).

### Co(111)-Ru<sub>7</sub>-4×4



Figure S6. Various structures and adsorption energies for  $Ru_7$  on the Co(111) surface (adsorption energy in eV).

# Co(111)-Ru<sub>8</sub>-4×4



Figure S7. Various structures and adsorption energies for  $Ru_8$  on the Co(111) surface (adsorption energy in eV).

### Co(111)-Ru<sub>9</sub>-4×4





# Co(111)-Ru<sub>9</sub>-5×5



Figure S8. Various structures and adsorption energies for  $Ru_9$  on the Co(111) surface (adsorption energy in eV).

## Co(111)-Ru<sub>10</sub>-5×5



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).

Co(311)-Ru<sub>4</sub>-4×4



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

### Co(311)-Ru<sub>6</sub>-4×4



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  $Ru_{11}$  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.