Supporting Information

Adsorption of Au_n (n = 1-4) clusters on Fe_3O_4(001) B-termination

Xiaohu Yu,[a,b] Xuemei Zhang,[b]Shengguang Wang[b,c],Gang Feng[b,d,e]**

a)College of Physics and Electrical Engineering, Anyang Normal University, Anyang, Henan, 455000, People's Republic of China; b) State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, Shanxi 030001, China; c) China Synfuels China Co., Ltd., Huairou, Beijing 101407, P.R. China; d) Shanghai Research Institute of Petrochemical Technology SINOPEC, 201208, Shanghai, P.R. China; e) *College of Chemistry, Nanchang University, Nanchang, Jiangxi 330031 P.R. China;*

Corresponding authors:

Xiaohu Yu Tel:+86 372 2900041; fax: +86 372 2900041; Email: yuxiaohu950203@126.com

Gang Feng Tel:+86 21 68462197; fax:+86 21 68462283; Email: fengg.sshy@sinopec.com

Fig. S1. Stable configurations of single Au atom adsorption on stoichiometric $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)

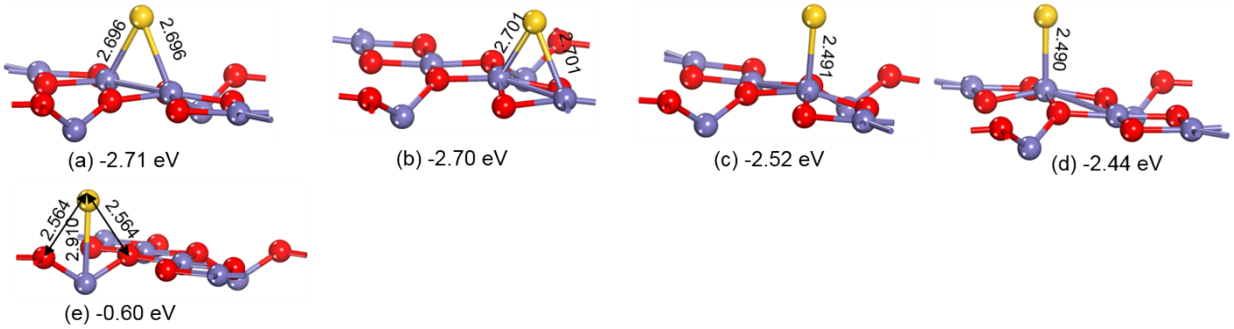


Fig. S2. Stable configurations of Au_2 dimer adsorption on stoichiometric $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)

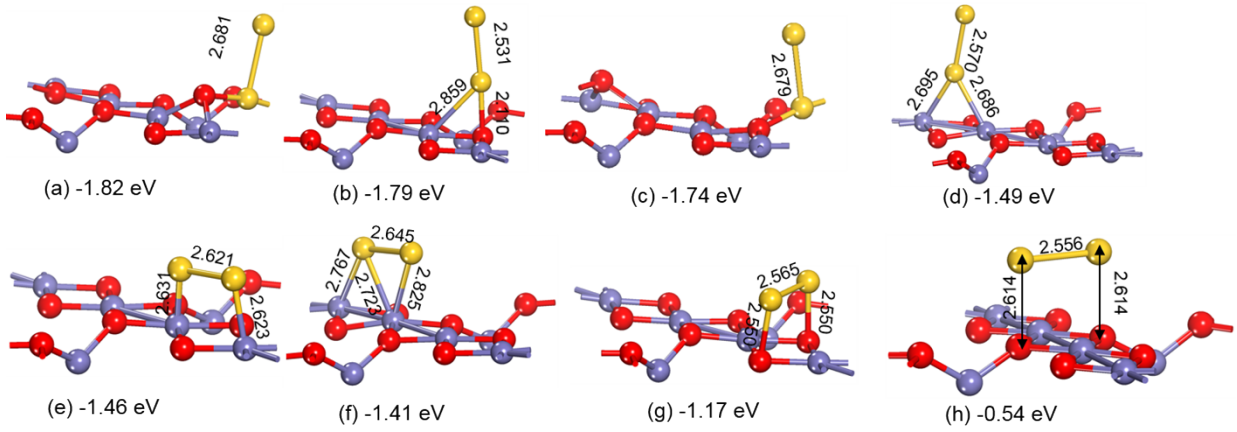


Fig. S3. Stable configurations of Au_3 trimer adsorption on stoichiometric $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)

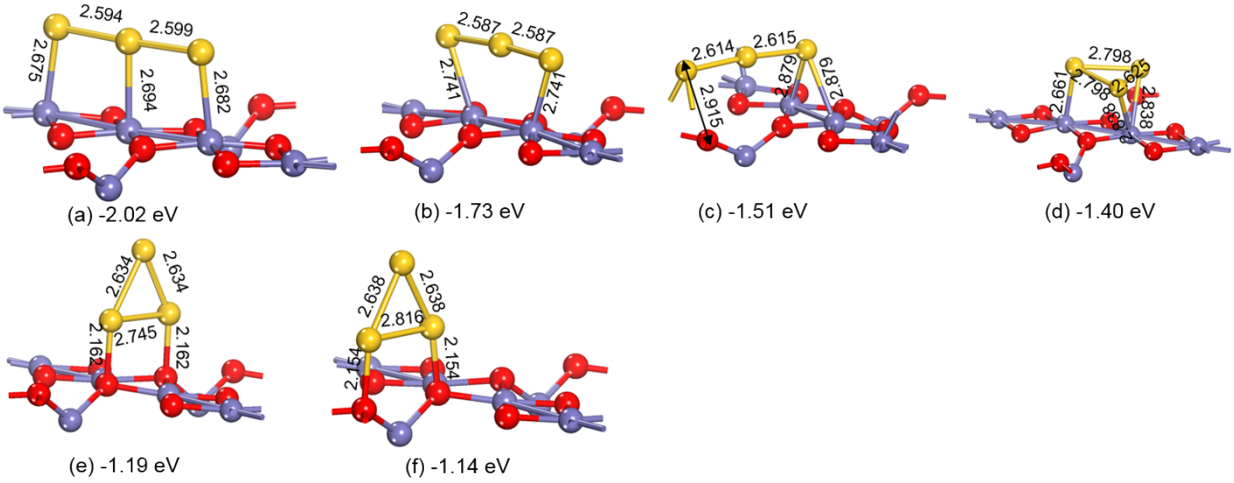


Fig. S4. Stable adsorption configurations of Au_4 tetramer adsorption on stoichiometric $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)

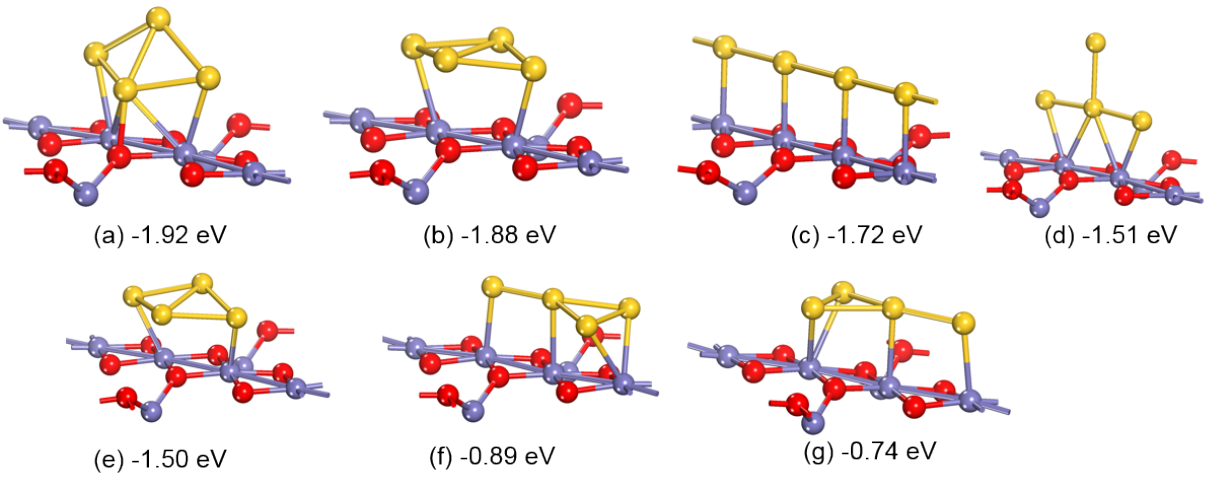
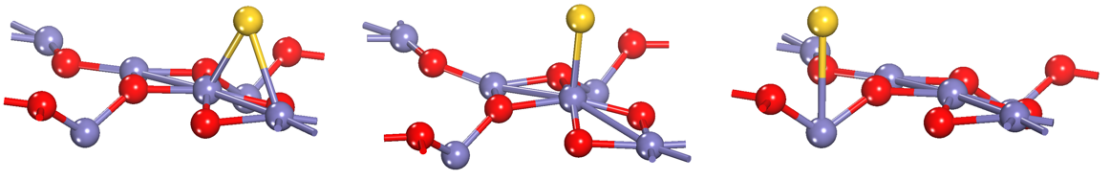
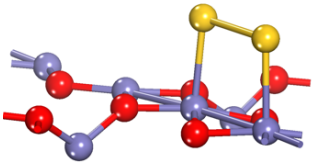


Fig. S5. Stable adsorption configurations of single Au atom adsorption on reduced Fe_3O_4(001) surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)



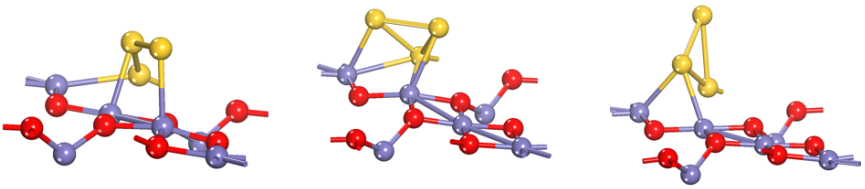
(a) -1.72 eV (b) -1.57 eV (c) -0.59 eV

Fig. S6. Stable adsorption configurations of Au_2 dimer adsorption on reduced Fe_3O_4(001) surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)



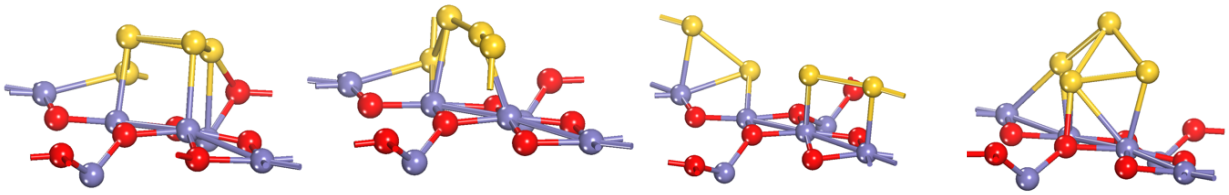
(a) -1.82 eV

Fig. S7. Stable adsorption configurations of Au_3 trimer adsorption on reduced $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)



(a) -3.25 eV (b) -2.79 eV (c) -1.60 eV

Fig. S8. Stable adsorption configurations of Au4 tetramer adsorption on reduced $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; yellow ball for gold atom)



(a) -2.28 eV (b) -2.24 eV (c) -1.58 eV (d) -0.02 eV

Fig. S9. Stable adsorption configurations of single Au atom adsorption on hydrated $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; white ball for hydrogen atom and yellow ball for gold atom)

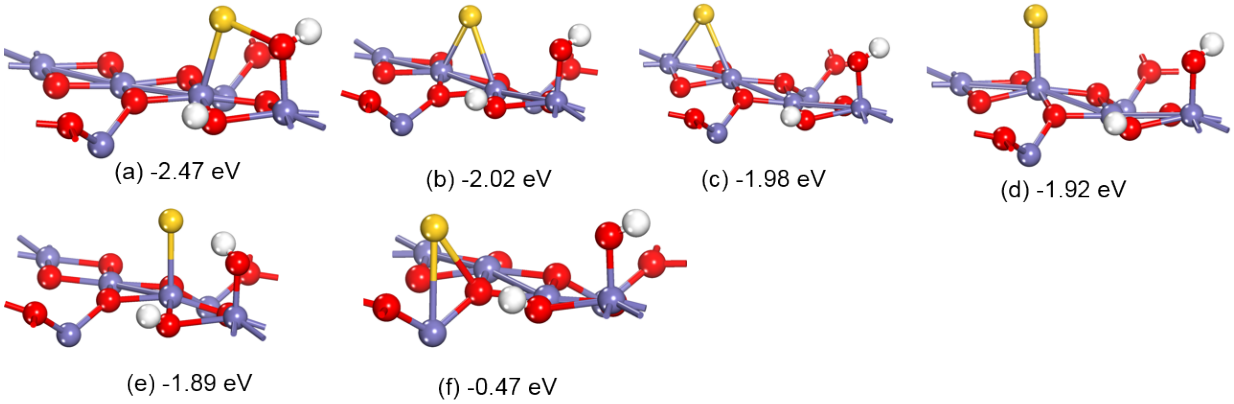


Fig. S10. Stable adsorption configurations of Au_2 dimer adsorption on hydrated $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; white ball for hydrogen atom and yellow ball for gold atom)

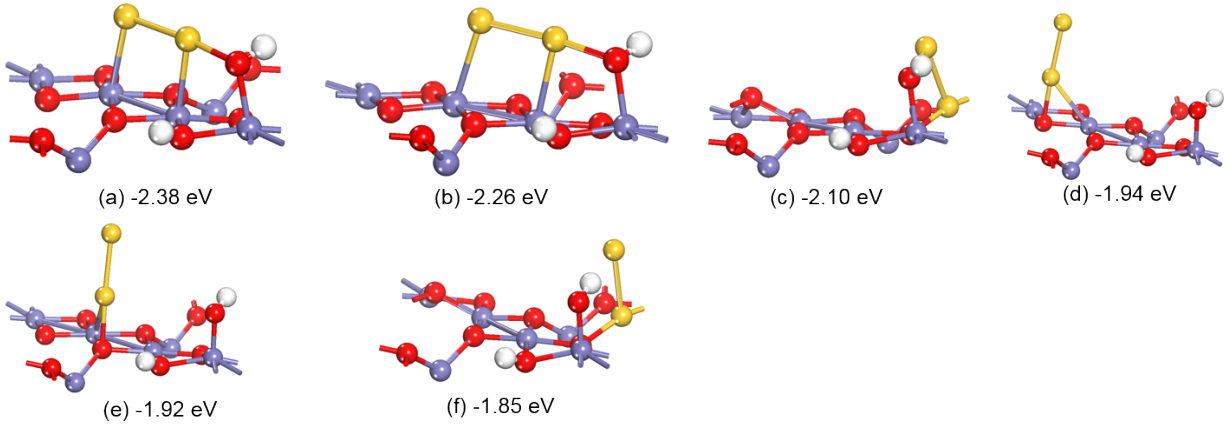


Fig. S11. Stable adsorption configurations of Au_3 trimer adsorption on hydrated $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; white ball for hydrogen atom and yellow ball for gold atom)

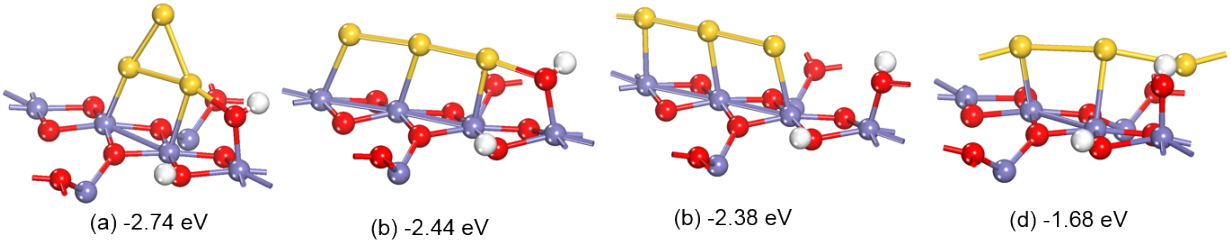


Fig. S12. Stable adsorption configurations of Au_4 tetramer adsorption on hydrated $Fe_3O_4(001)$ surface. (red ball for oxygen atom; blue ball for iron atom; white ball for hydrogen atom and yellow ball for gold atom)

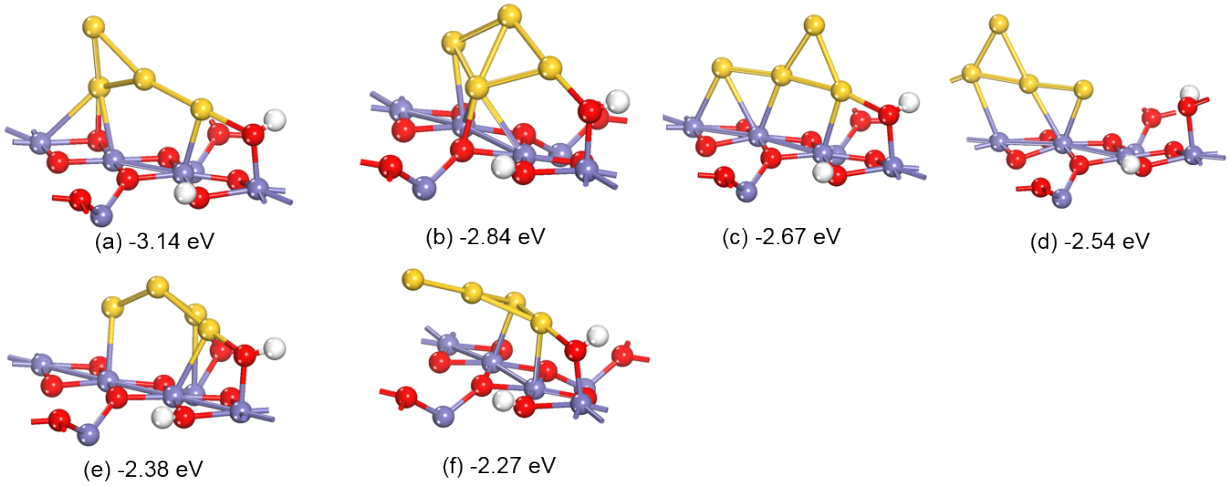
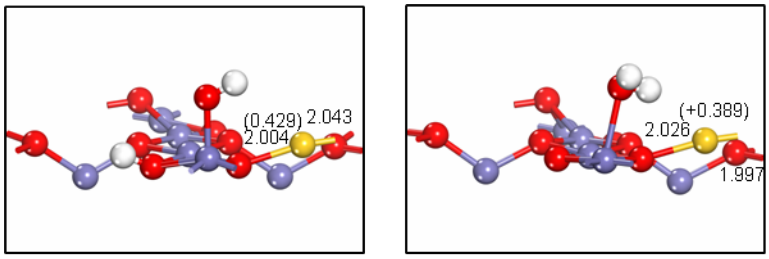


Fig. S13. Hydrogen spillover on the hydrated Fe_3O_4(001) B-termination with adsorption energy (eV), Au-Fe distances (Å), and the Bader charge of Au atoms (in parenthesis) (red ball for oxygen atom; blue ball for iron atom and yellow ball for gold atom)



(a) -3.16 eV (b) -2.05 eV

Fig. S14. The most stable atomic Au adsorption configurations on the Fe_3O_4(001) B-termination (A) stoichiometric surface; (B) reduced surface; (C) hydrated surface, with adsorption energy (eV), Au-Fe distances (Å), and the Bader charge of Au atoms (in parenthesis) (red ball for oxygen atom; blue ball for iron atom and yellow ball for gold atom)

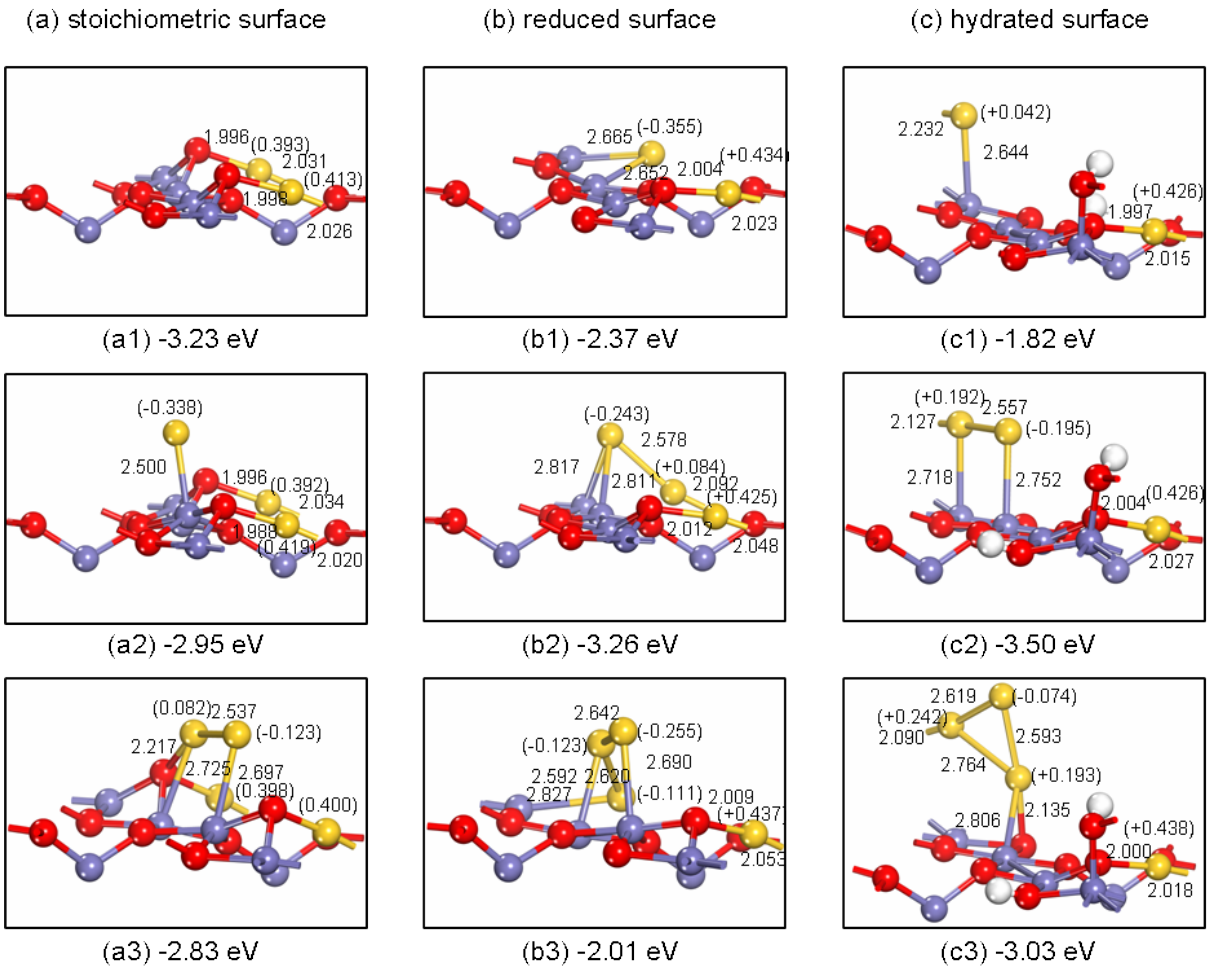


Fig. S15. Magnetic moments of Fe atoms for Au_n (n=2-4) adsorption on the surfaces. (red ball for oxygen atom; blue ball for iron atom; white ball for hydrogen atom and yellow ball for gold atom)