Supporting Information for

Carbon Chain Growth by Formyl Coupling over Cu/γ-AlOOH (001) surface in Syngas Conversion

Hui Bai,*[a,b] Mengmeng Ma,[a] Bing Bai,[a,b] Haojie Cao,[a] Lin Zhang,[a] Zhihua Gao,[a] Vladimir A. Vinokurov[c] and Wei Huang*[a]

[a]*Key Laboratory of Coal Science and Technology of Ministry of Education and Shanxi Province, Taiyuan University of Technology, Taiyuan 030024, China.*

[b]*Department of Chemistry, Brown University, Providence, RI 02912, USA*

[c]*Department of Physical and Colloid Chemistry, Gubkin Russian State University of Oil and Gas (National Research University), Leninskiy prospect 65/1, Moscow, 119991, Russia*

*Corresponding authors:

E-mail addresses: baihui@tyut.edu.cn; huangwei@tyut.edu.cn;

Figure S1 The most stable adsorption configurations of possible species involved in the pathways of syngas-to-ethanol conversion over Cu/γ-AlOOH (001) surface. Gray spheres represent C atoms, light blue spheres represent H atoms from H_2 and brown spheres represent O atoms from CO.

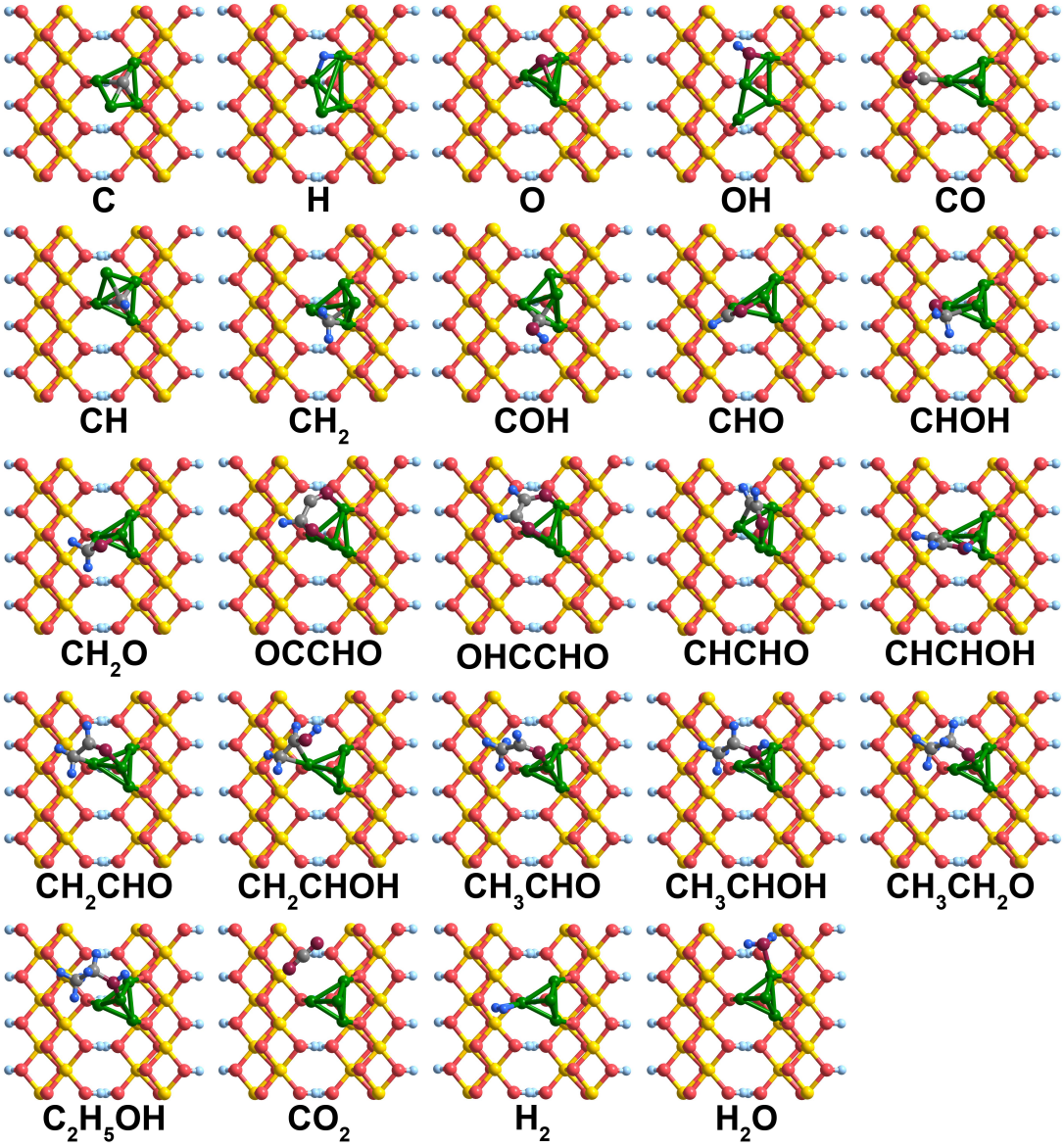

Figure S2 The potential energy profile for OHCCHO hydrogenation with the structures of initial states (ISs), transition states (TSs), and final states (FSs).

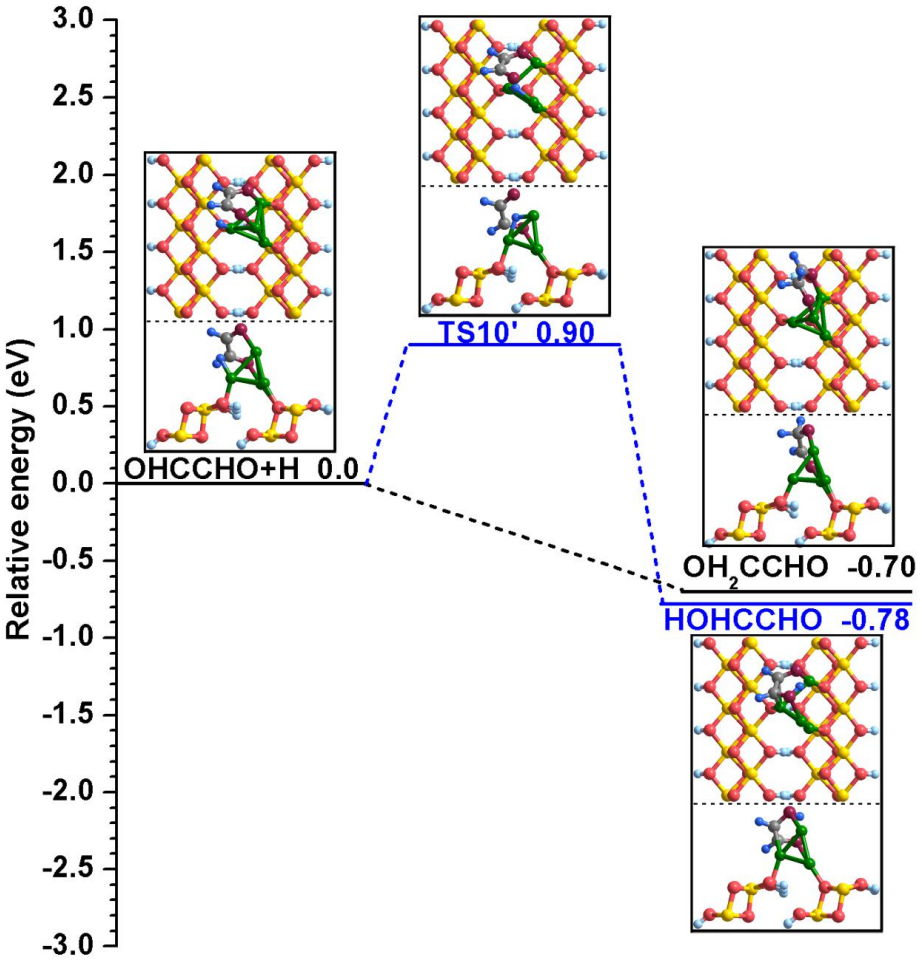

Figure S3 The potential energy profile for OH_2CCHO hydrogenation with the structures of initial states (ISs), transition states (TSs), and final states (FSs).

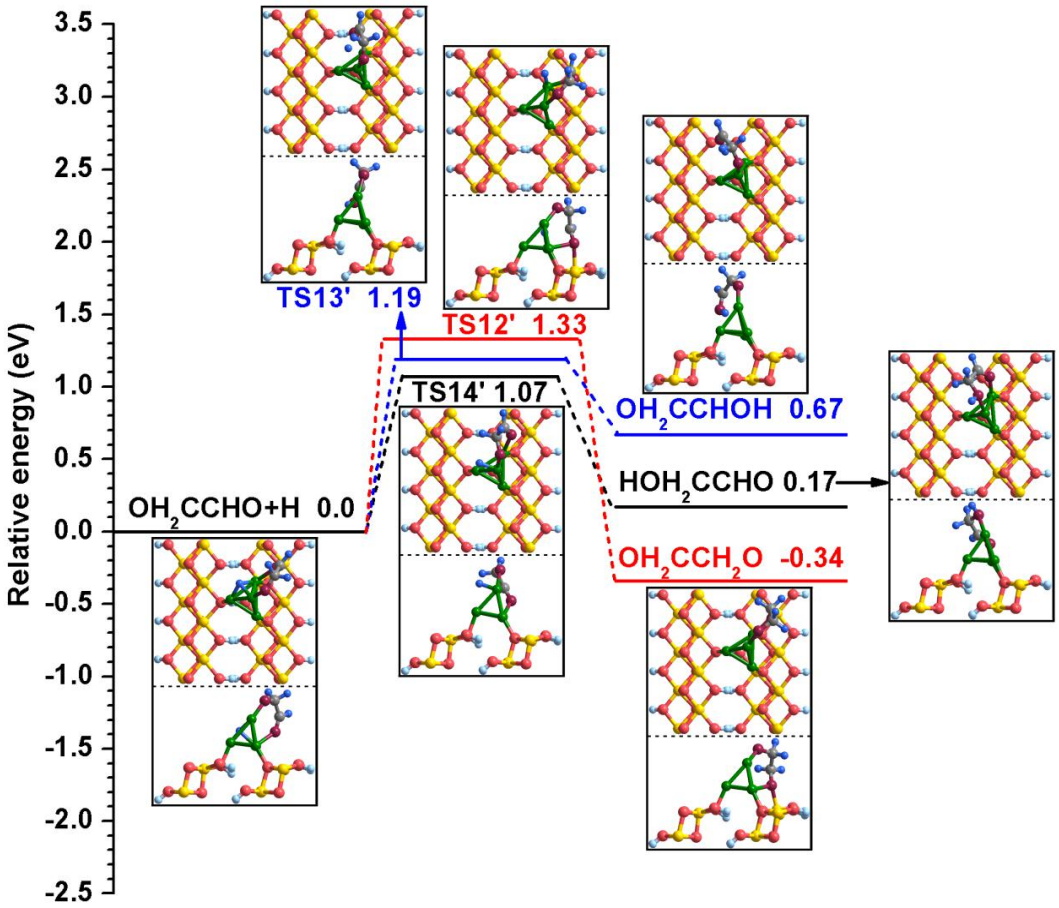

Figure S4 The potential energy profile for (a) HOH_2CCHO hydrogenation and (b) HOH_2CCH_2OH formation with the structures of initial states (ISs), transition states (TSs), and final states (FSs).