Supporting Information

CO_2 formation mechanism in Fischer-Tropsch synthesis over iron-based catalysts: A combined experimental and theoretical study

*Bing Liu,† Wenping Li,† Jiao Zheng, Qiang Lin, Xin Zhang, Junwei Zhang, Feng Jiang, Yuebing Xu and Xiaohao Liu**

Department of Chemical Engineering, School of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, P. R. China

† These authors contributed equally to this work

* Corresponding author:

Email: liuxh@jiangnan.edu.cn (X.L)

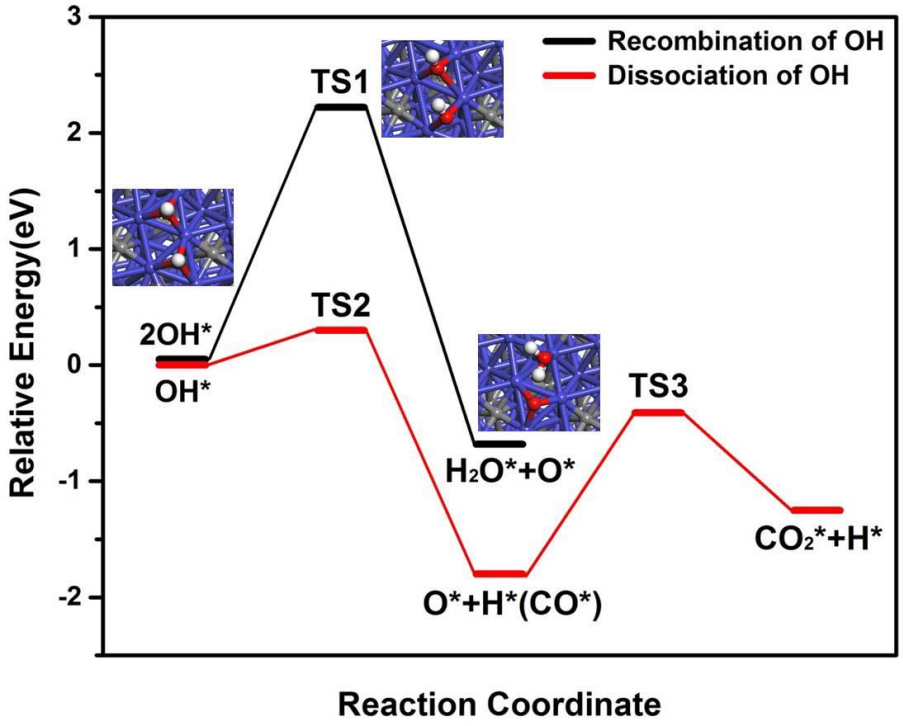

Figure S1. Energy profiles for the recombination of 2OH to form H_2O and the dissociation of OH to form CO_2 over χ-Fe_5C_2(510).

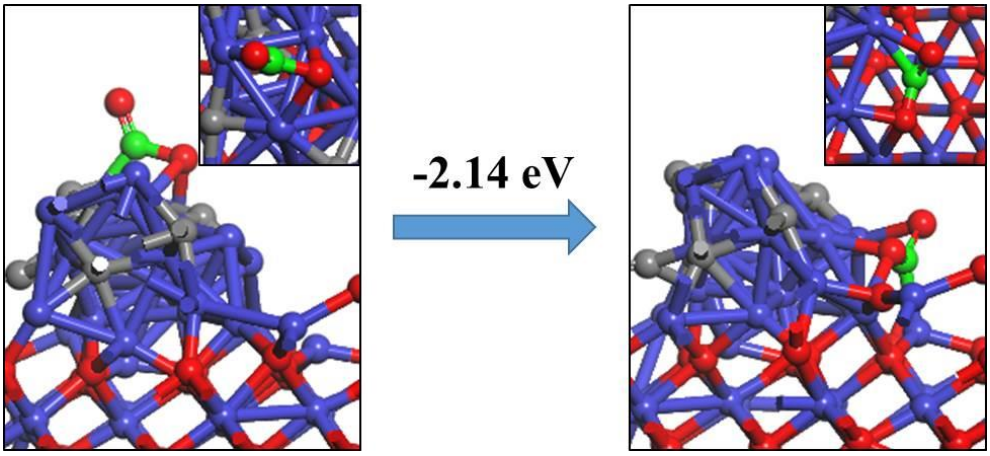

Figure S2. CO_2 spillover from Fe_5C_2 to Fe_3O_4 and the corresponding energy.

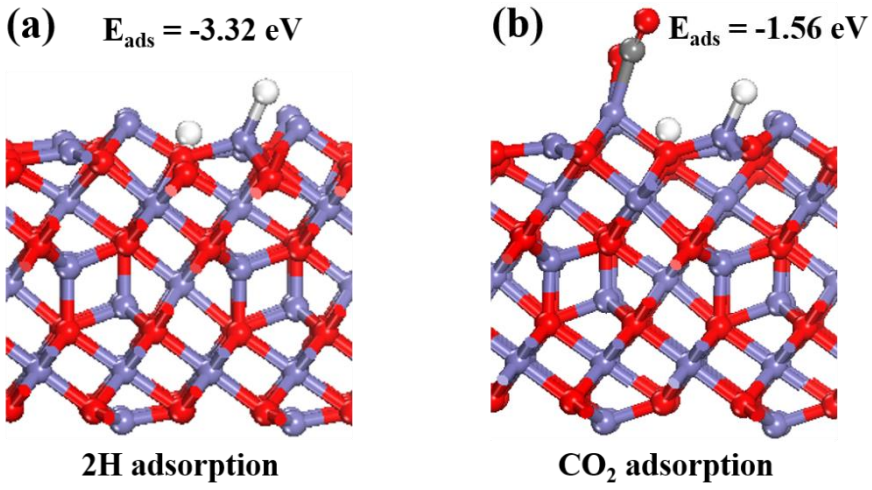

Figure S3. Adsorption energies for 2H and CO_2 over Fe_3O_4(111) surface.

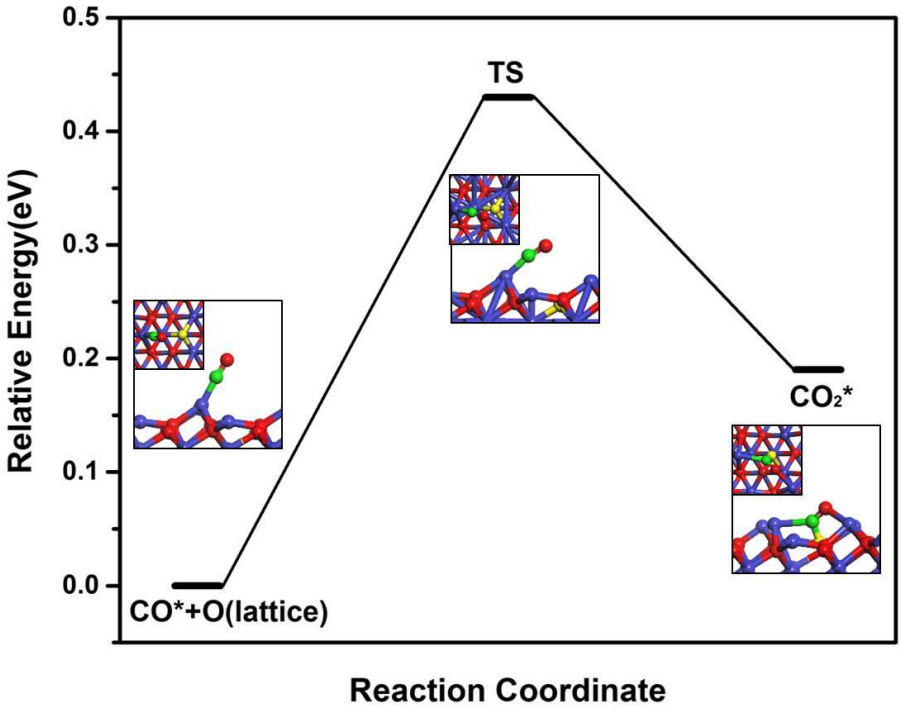

Figure S4. CO_2 formation through the reaction between CO and lattice O in $Fe_3O_4(111)$.