**Supplementary Information**

**The Reverse Water Gas Shift Reaction (RWGS) Mechanism Study on γ-MoC(100) Surface**

Xiaoshu Yao, Zhihong Wei\*, Jingyuan Mei, Xianhui Guo, Xinxin Tian\*

Institute of Molecular Science, Key Laboratory of Materials for Energy Conversion and Storage of Shanxi Province and Key Laboratory of Chemical Biology and Molecular Engineering of Ministry of Education, Shanxi University, Taiyuan 030006, China

E-mail: weizhihong@sxu.edu.cn, tianxx@sxu.edu.cn

Table S1 The calculated vibration frequencies (ωe, cm-1) of CO2, H2, CO, H2O, COOH and HCOO species.

|  |  |
| --- | --- |
| **Species** | **Frequencies (cm-1 )** |
| CO2 | 1247.069467 |
| 969.514423 |
| H2 | 2710.624841 |
| 1487.210506 |
| 907.409090 |
| CO | 1131.829240 |
| H2O | 3550.495684 |
| 3425.004868 |
| 1455.795720 |
| OH | 3582.015263 |
| COOH | 3516.288128 |
| 1151.455300 |
| HCOO | 3022.856100 |
| 1307.436108 |
| 1133.844107 |
| 1094.765419 |

Fig. S1 The possible adsorption configuration of CO3 intermediate on the γ-MoC(100) surface.



Fig. S2 The HUMO and LUMO orbitals of the bent (V-shaped) CO2.

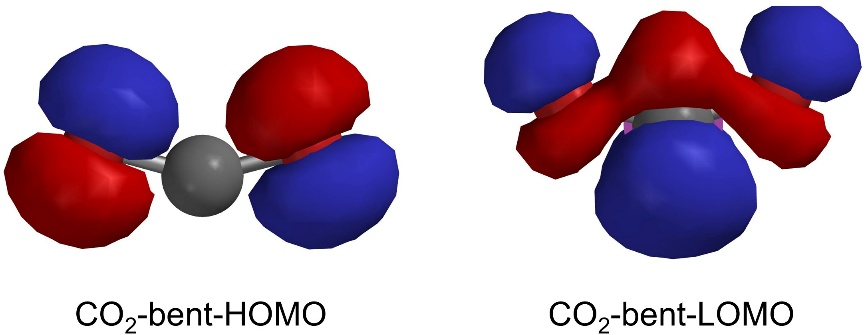


Fig. S3 Projected density of states (PDOS) for γ-MoC(100) and α-MoC(111) surfaces.

