Supporting Information

Carbonate-mediated Mars-van Krevelen mechanism for CO oxidation on cobalt-doped ceria catalysts: Facet-dependence and coordination-dependence

Bing Liu,*1 Wenping Li,1 Weiyu Song,2 Jian Liu*2

1Department of Chemical Engineering, School of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, P. R. China

2State Key Laboratory of Heavy Oil Processing, College of Science, China University of Petroleum-Beijing, Beijing 102249, P. R. China

* Corresponding author:
Email:  liubing@jiangnan.edu.cn (B.L.); liujian@cup.edu.cn (J.L.)
Figure S1. Calculated structures in the conventional M-vK mechanism for CO oxidation on Co-CeO$_2$(110).
Figure S2. Energy profile and corresponding structures for carbonate dissociation via bicarbonate route.
Figure S3. Calculated structures in the carbonate-mediated M-vK mechanism for CO oxidation on Co-CeO$_2$(111).
Figure S4. Calculated structures in the carbonate-mediated M-vK mechanism for CO oxidation on Co-CeO$_2$(100).