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Supporting Information

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

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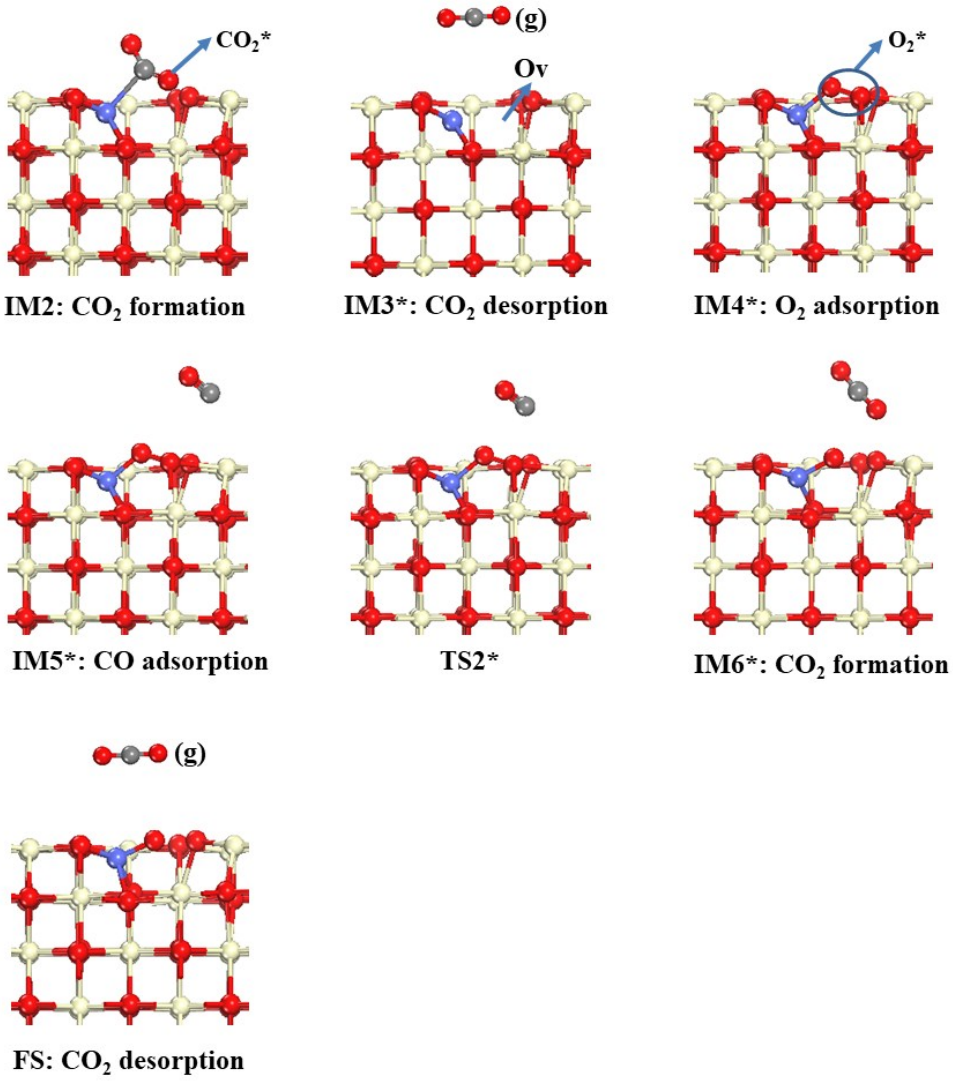

Figure S1. Calculated structures in the conventional M-vK mechanism for CO oxidation on Co-CeO_2(110).

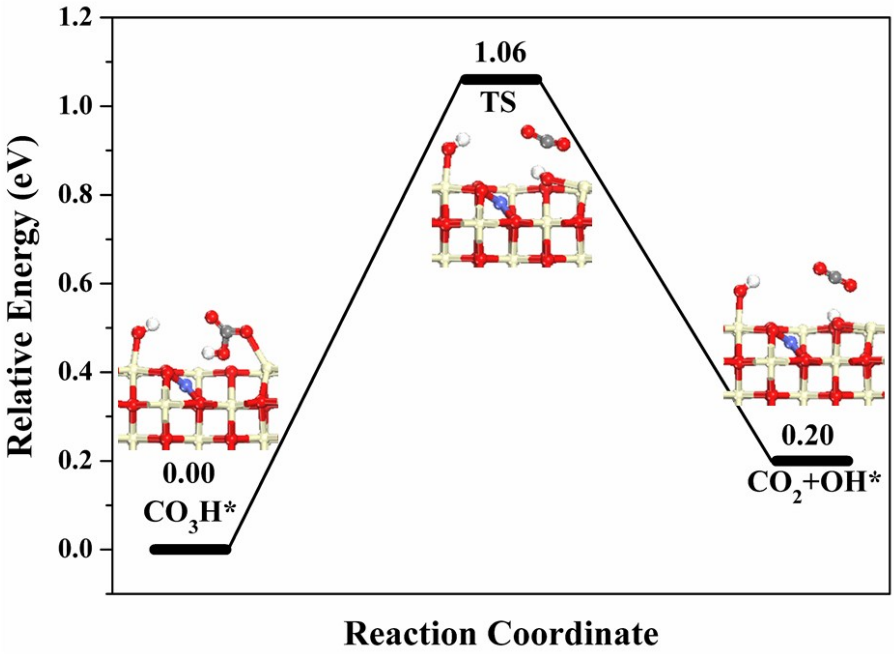

Figure S2. Energy profile and corresponding structures for carbonate dissociation via bicarbonate route.

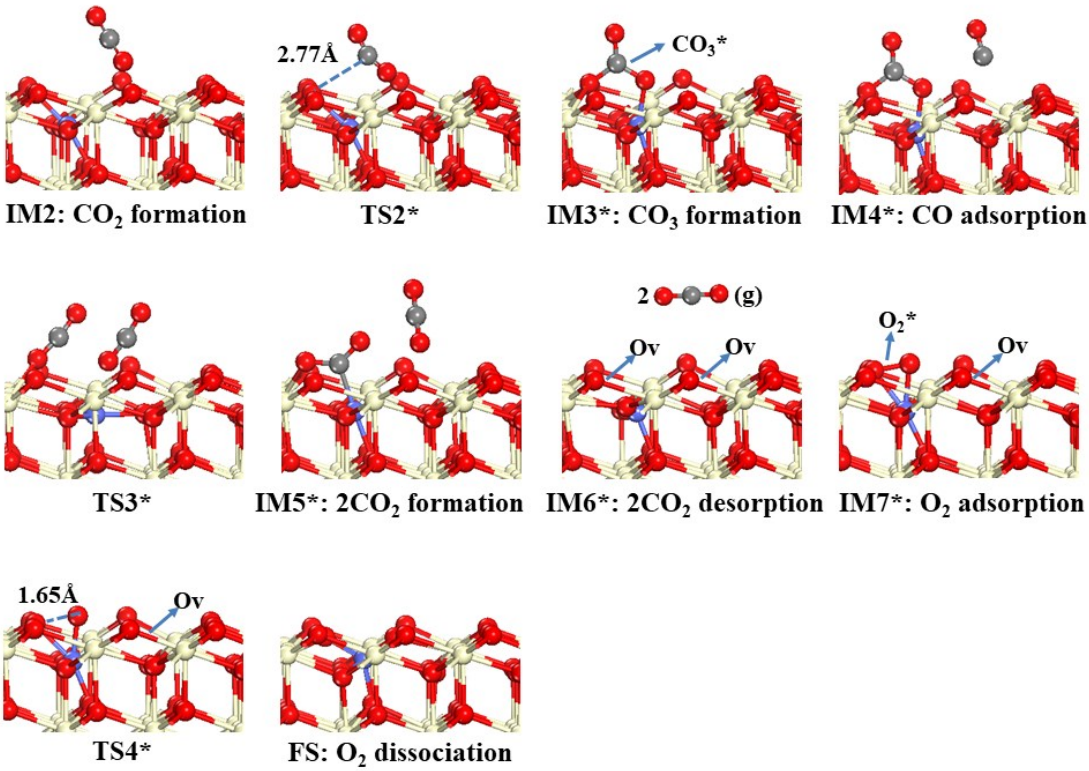

Figure S3. Calculated structures in the carbonate-mediated M-vK mechanism for CO oxidation on Co-CeO_2(111).

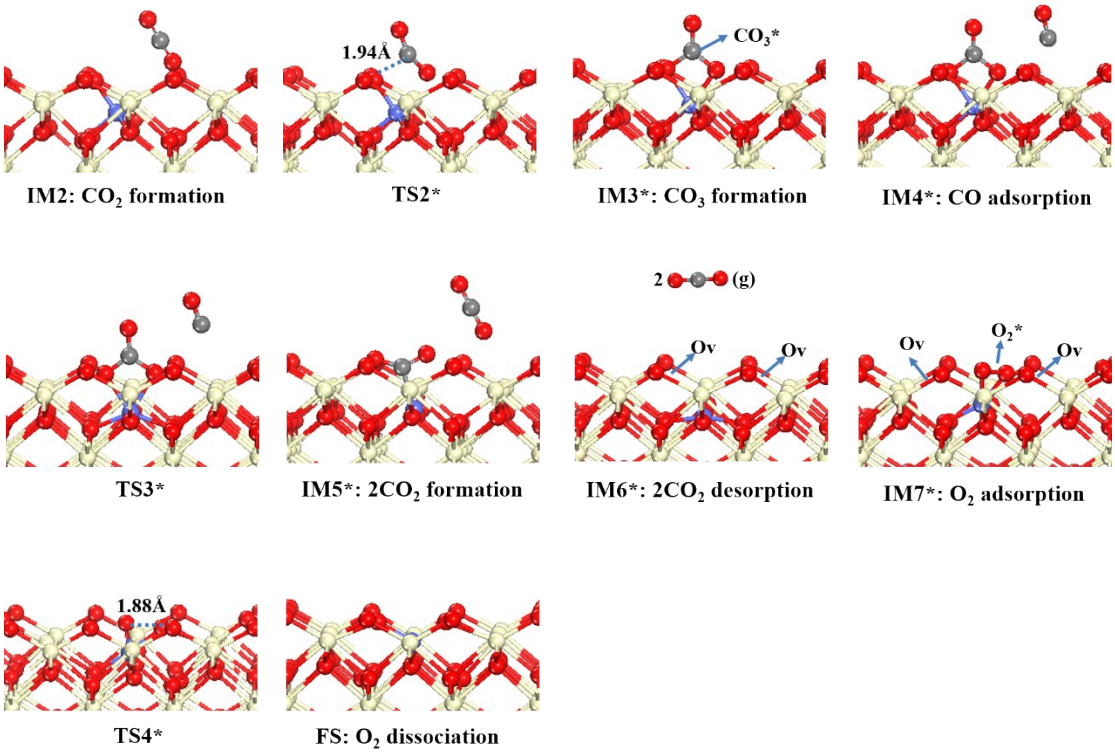

Figure S4. Calculated structures in the carbonate-mediated M-vK mechanism for CO oxidation on Co-CeO_2(100).