Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary for

Mechanistic Insight into Methane Dry Reforming over Cobalt: A Density Functional Theory Study

Heyuan Huang,[ab] Yingzhe Yu,[ab] and Minhua Zhang* [ab]

Table S1. The elementary processes and corresponding kinetic parameters for DRM over Co(0001)

Elementary processes	$E_{a,f}$ *(eV)*	$E_{a,r}$ (eV)	$v_{0,f}$ (s^{-1})	$v_{0,r}$ (s^{-1})
$CH_4(g) + 2* \rightarrow CH_3* + H*$	0.95	1.07	2.62E+9	5.50E+13
$CH_3* + * \rightarrow CH_2* + H*$	0.78	0.65	3.94E+13	2.69E+13
$CH_2* + H* \rightarrow CH* + *$	0.28	0.67	1.62E+13	1.03E+13
$CH* + * \rightarrow C* + H*$	1.15	0.82	2.29E+13	3.46E+13
$CO_2(g)+*\rightarrow CO*+O*$	0.26	1.47	9.83E+8	6.98E+13
$CO_2* + H*$ = *trans*-COOH* + *	1.15	1.16	1.97E+13	8.56E+13
trans-COOH* = *cis*-COOH*	0.79	0.50	2.17E+13	6.04E+13
cis-COOH* + * = CO* +OH*	0.29	1.66	2.71E+13	6.53E+13
$CH_3* + O* = CH_3O* +*$	1.99	1.50	4.39E+13	5.37E+13
$CH_2* +O* = CH_2O* + *$	1.97	1.32	8.49E+12	4.38E+12
$CH* + O* = CHO* + *$	1.34	0.68	8.77E+12	1.43E+13
$C* + O* = CO* + *$	1.64	2.53	7.29E+13	1.12E+13
$CH_3* + OH* = CH_3OH* + *$	2.37	1.60	6.38E+12	9.38E+12
$CH_2* + OH* = CH_2OH*$	1.57	0.84	9.64E+12	1.08E+12
$CH* + OH* = CHOH* + *$	1.88	1.07	4.36E+12	7.86E+12
$C* + OH* = COH* + *$	1.27	1.52	6.72E+12	9.82E+12
$CH_3OH* + * = CH_2OH* + H*$	1.16	1.04	3.82E+13	1.92E+13
$CH_2OH* +* = CHOH* + H*$	0.62	0.94	9.81E+12	8.92E+12
$CHOH* + *= COH* + H*$	0.07	0.83	1.07E+13	2.45E+13
$COH* +* = CO* + H*$	0.95	1.20	2.38E+13	6.74E+12
$CH_3OH* +* = CH_3O* + H*$	0.93	1.64	2.32E+13	4.31E+13
$CH_2OH* +* = CH_2O*+ H*$	0.57	0.89	1.92E+12	9.28E+12
$CHOH* +* = CHO*+ H*$	1.05	1.42	4.35E+13	2.85E+13
$CH_3O* +* = CH_2O* + H*$	0.98	0.54	1.76E+13	1.27E+13
$CH_2O* +* = CHO* + H*$	0.42	0.74	3.87E+13	2.81E+13
$CHO* +* = CO*+H*$	0.16	1.34	2.21E+13	8.81E+12
$O*+H* = *OH*+*$	1.37	1.05	1.31E+13	1.42E+14
$OH*+H* = H_2O*+*$	1.50	0.85	2.68E+14	1.95E+14
$OH*+OH* = H_2O*+O*$	0.98	0.70	2.29E+13	2.03E+13
$2H* = H_2*+*$	1.00	1.14	8.78E+12	1.82E+13

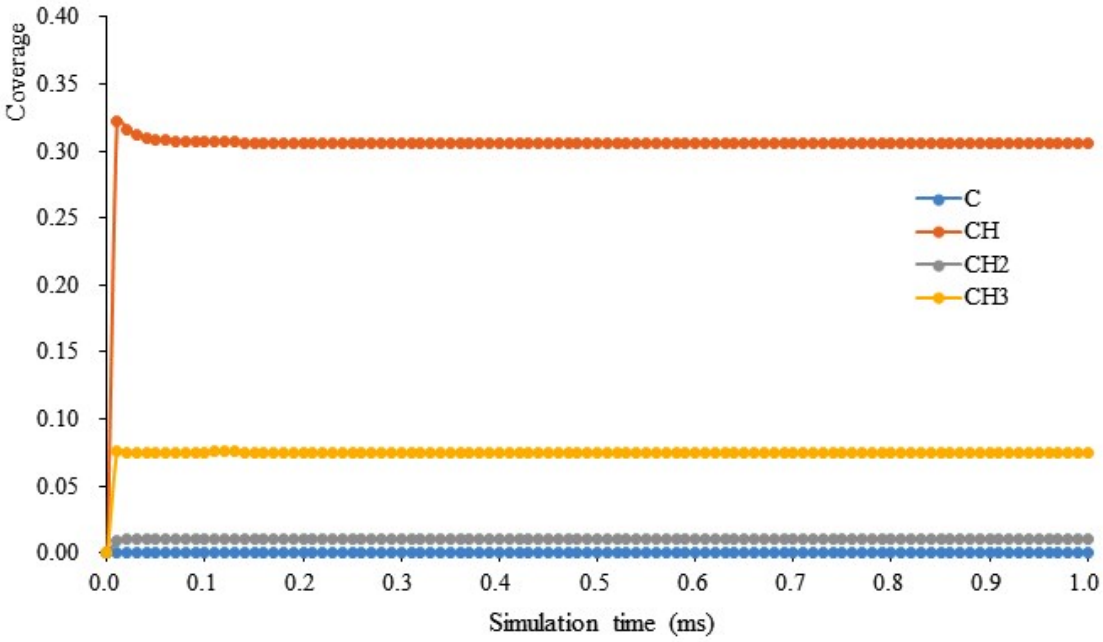

Fig. S1. The change of coverage of CH_x(x=0-3) over time within 1.0 ms simulation time on Co(0001)