Supporting information

Co-embedded sulfur vacant MoS$_2$ monolayer as a promising catalyst for formaldehyde

oxidation: a theoretical evaluation

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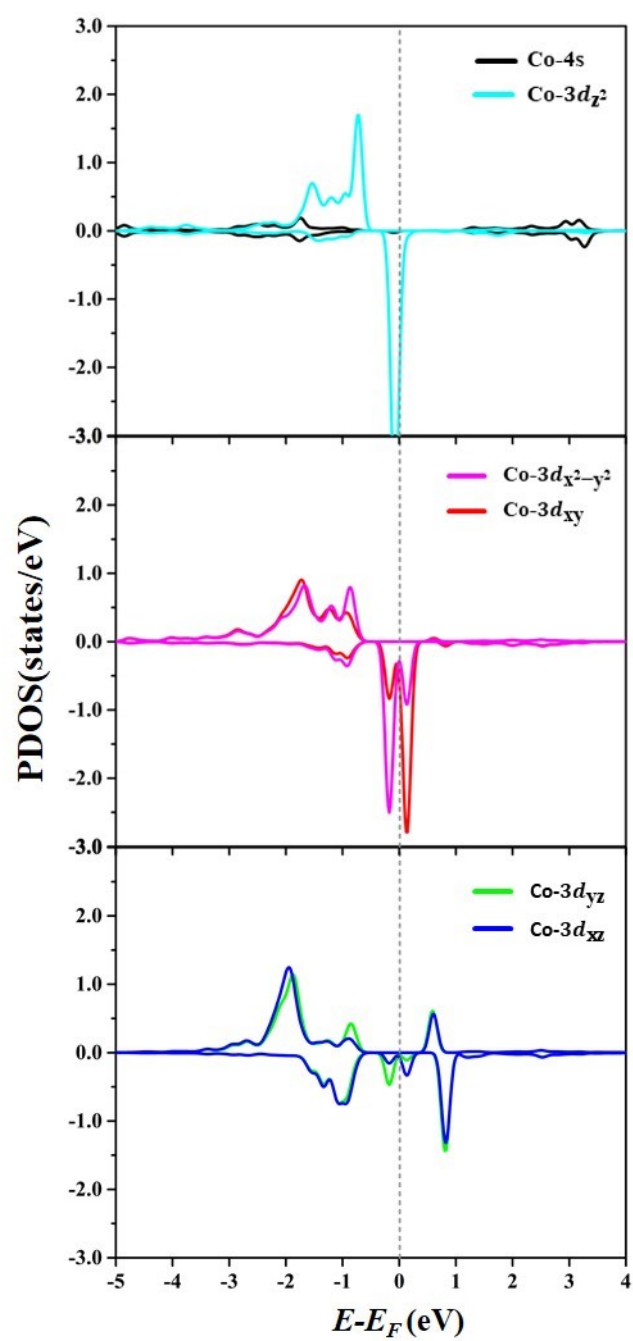
Figure S1. Projected density of state for the Co $4s$, $3d_{z^2}$, $3d_{x^2-y^2}$, $3d_{xy}$, $3d_{yz}$, $3d_{xz}$ in the
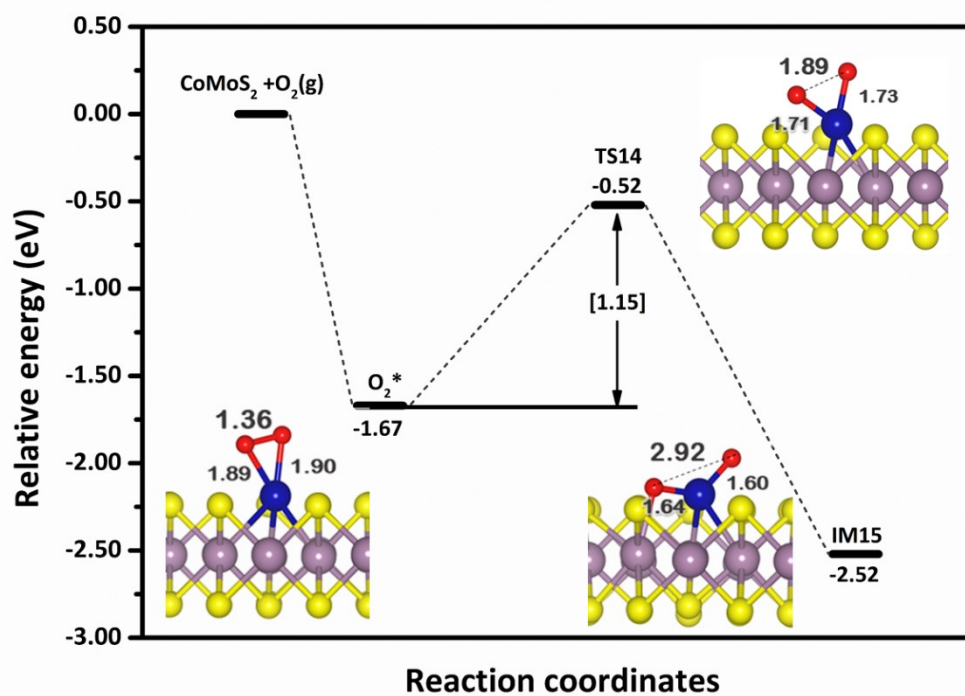
Co_{Sv}-MoS_2

Figure S2. Energy profile and corresponding structures of O_2 dissociation.

$E_{ads} = -1.50$ eV

(a)

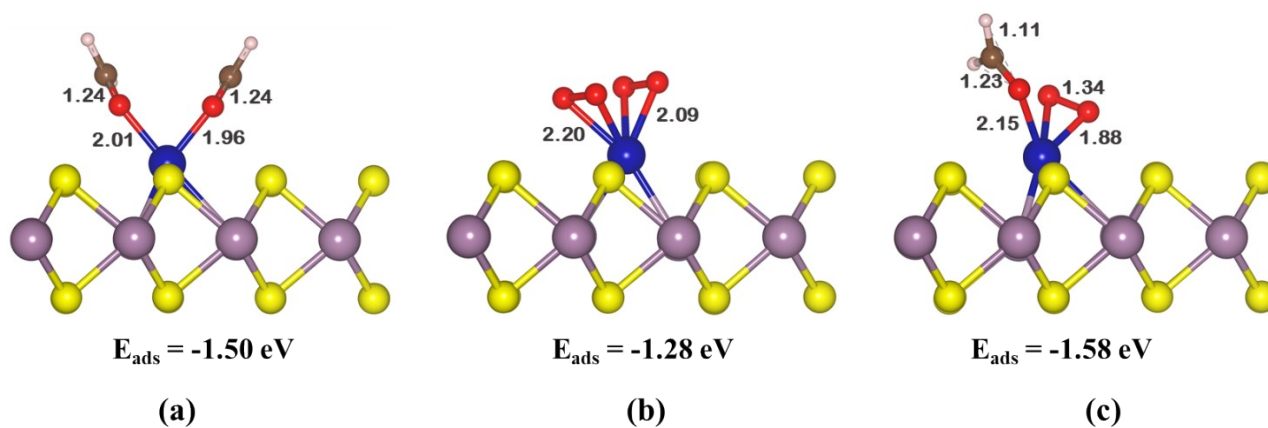$E_{ads} = -1.28$ eV

(b)

$E_{ads} = -1.58$ eV

(c)

Figure S3. The possible co-adsorption configurations between HCHO and O_2 on Co-MoS$_2$

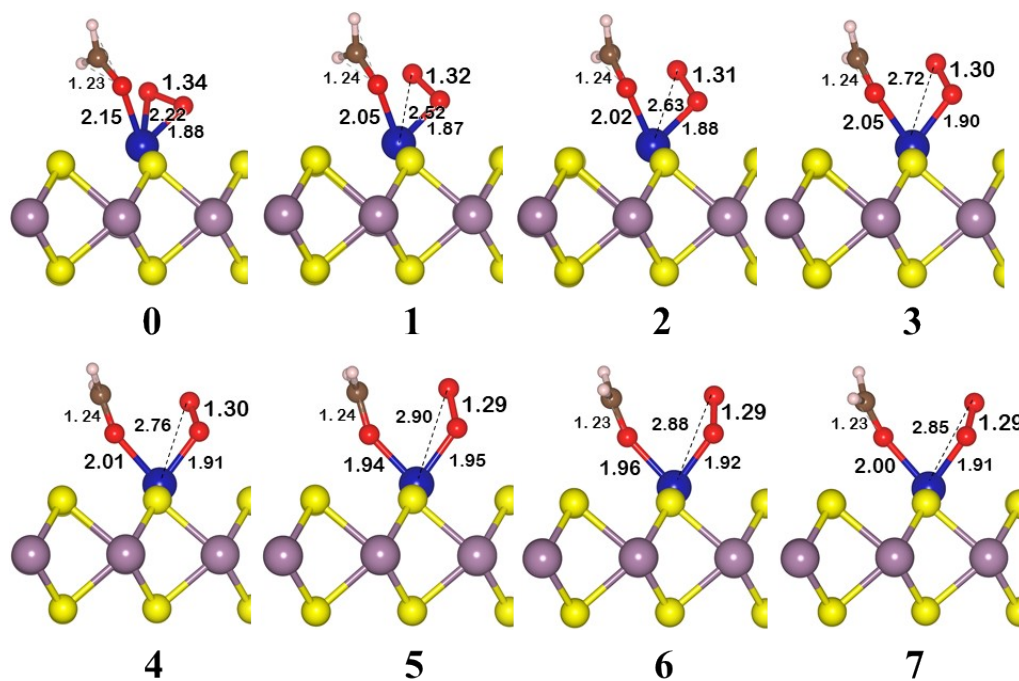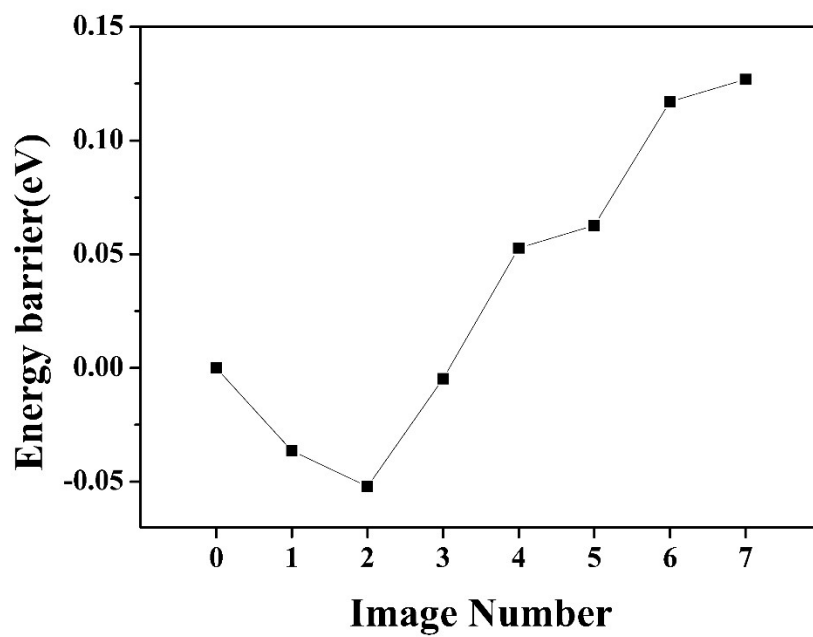(a) two-HCHO (b) two- O_2 (c) one-HCHO and one- O_2

Figure S4. Energy barrier and corresponding structures of IM6 to IM7

Table S1. Gibbs free energy barrier (ΔG_b, eV) and The reaction rate constants (k^{TST}) for

Species	E	E_b	E_{ZPE}	TS	$C_p dT$	G	G_b	k^{TST}
IM9→	-391.028		3.511	3.314	1.861	-388.970		
		0.312					0.32	2.04×10^7
TS9	-390.716		3.477	3.231	1.823	-388.646		
IM12→	-393.767		3.490	3.380	1.885	-391.773		
		0.301					0.34	1.26×10^7
TS11	-393.466		3.483	3.316	1.864	-391.436		
IM13→	-393.662		3.448	3.398	1.887	-391.724		
		0.414					0.42	4.97×10^5
TS12	-393.248		3.458	3.391	1.877	-391.304		
IM14→	-393.384		3.443	3.348	1.879	-391.410		
		0.380					0.31	3.46×10^7
TS13	-393.004		3.352	3.318	1.871	-391.100		

elementary steps of the co-adsorption path at 298.15 K.
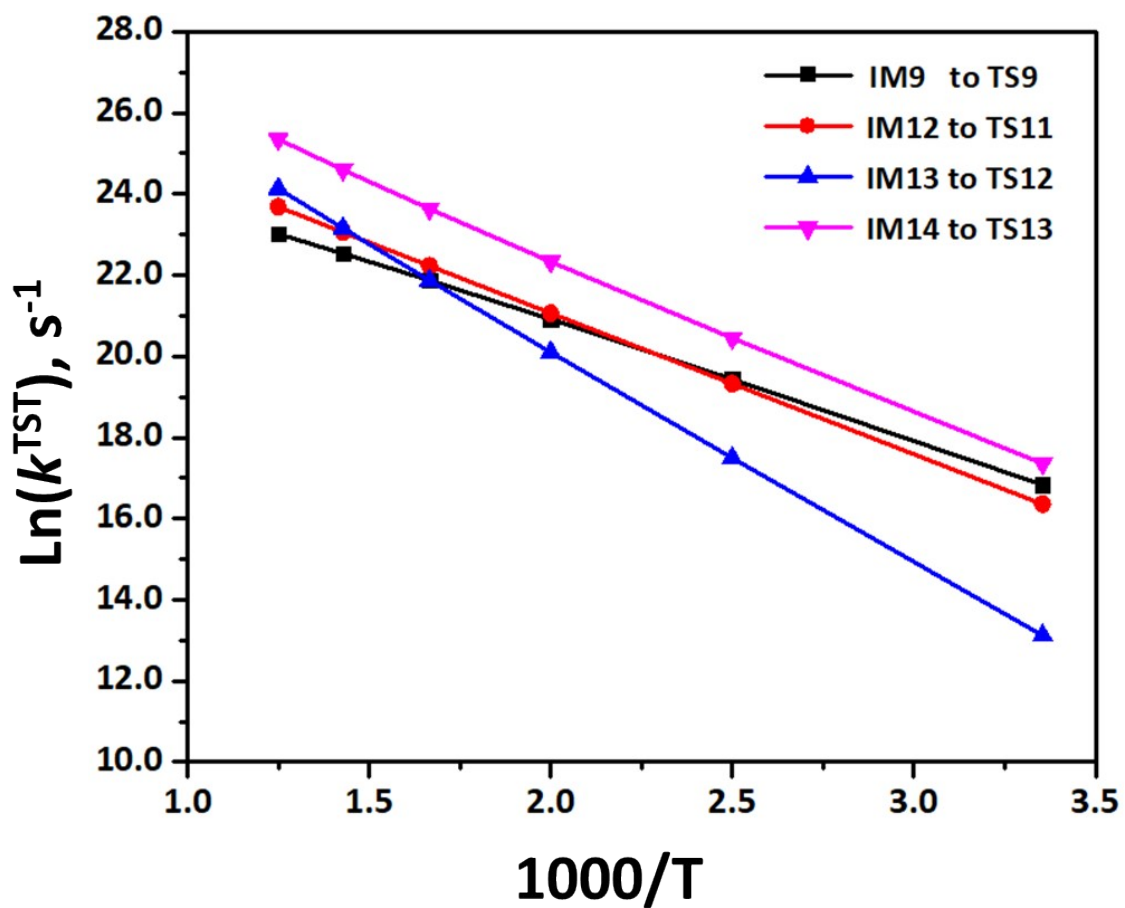
Figure S5. The logarithms of reaction rate constants for rate-determining steps of each elementary step at different temperatures (298.15 – 800 K).

Table S2. The reaction rate constants (k^{TST}) and Gibbs free energy barrier (ΔG_b) for rate-determining steps of each path at different temperatures.

Temperature (K)	Consecutive path		Co-adsorption path	
	k^{TST} (s^{-1})	ΔG_b eV(kJ.mol^{-1})	k^{Desorp} (s^{-1})	ΔG_b eV(kJ.mol^{-1})
298.15	1.12 x 10^5	0.46 (44.38)	1.99 x 10^0	0.74 (71.30)
400.00	1.03 x 10^8	0.39 (37.63)	2.08 x 10^4	0.68 (65.86)
500.00	6.34 x 10^9	0.32 (30.88)	4.07 x 10^6	0.64 (61.32)
600.00	1.06 x 10^{11}	0.25 (24.12)	1.24 x 10^8	0.60 (57.45)
700.00	8.28 x 10^{11}	0.17 (16.40)	1.32 x 10^9	0.46 (54.17)
800.00	4.00 x 10^{12}	0.10 (9.65)	7.91 x 10^9	0.53 (50.89)

System	Magnetic moment of Co in the system (μB)
Co_{Sv}-MoS$_2$	1.3
R1. HCHO direct decomposition	
HCHO*	0.2
CH$_2$* + O* (IM1)	0.9
CHO* + H* (IM2)	0.4
CO* +2H* (FS1)	0.7
CO* (FS1')	1.2
R2. CO oxidation	
CO* + O$_2$* (IM3)	1.6
OCOO* (IM4)	1.1
O*	-0.4
CO$_2$ (FS3)	1.3
R3. HCHO oxidation by O$_2$	
HCHO* + O$_2$* (IM6)	1.9
HCHO* + O$_2$* (IM7)	1.8
CHO* + OOH* (IM8)	1.2
OCH$_2$OO* (IM9)	2.0
HCOOH* + O* (IM10)	2.1
η^1-OCHO* + OH* (IM11)	2.2
η^2-OCHO* + OH* (IM13)	-2.3
η^1-OCHO* + OH* (IM4)	2.2
CO$_2$* + H$_2$O* (FS4)	1.4

Table S3. Calculated magnetic moments of Cobalt (Co) in the systems.