Supporting Information

Density Functional Theory Study of Methanol Steam Reforming on $Pt_3Sn(111)$ and the Promotion Effect of a Surface Hydroxy Group

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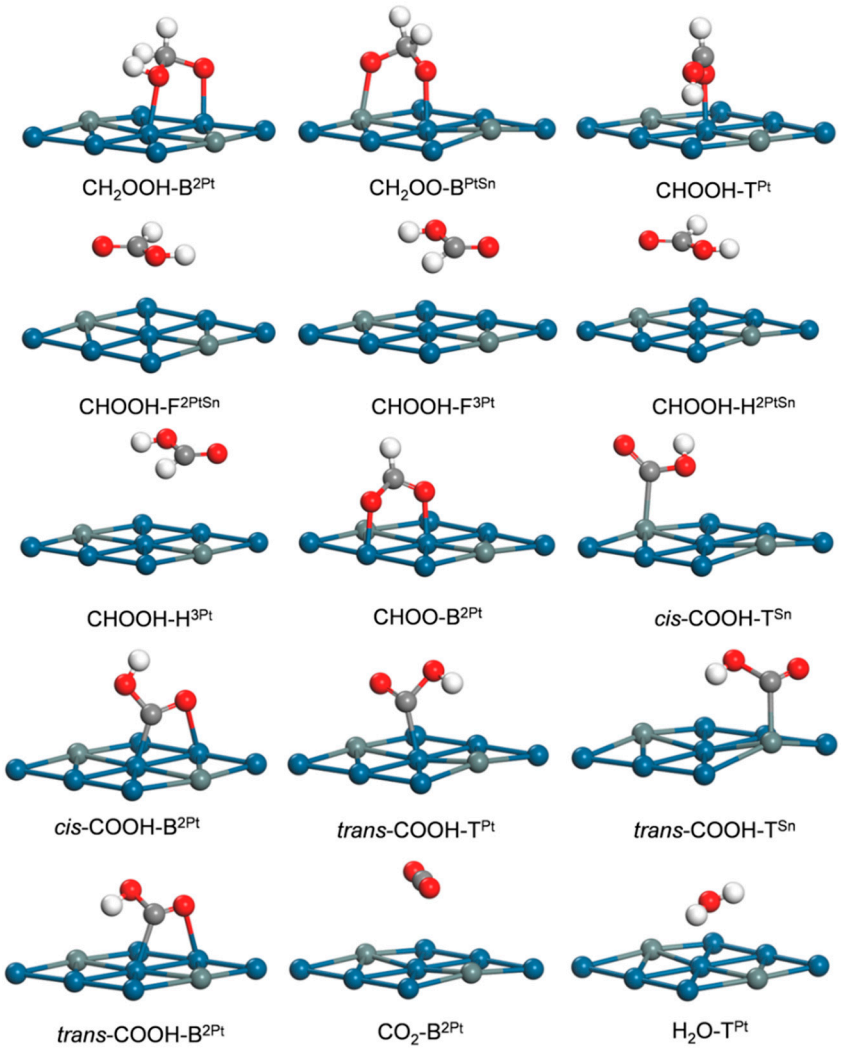

Figure S1. The other adsorption configurations of reaction intermediates along reaction pathway of Methanol Steam Reformation (MSR) to CO_2 on $Pt_3Sn(111)$.

Table S1. Sub-stable Adsorption Sites, Energies (in eV) and Structural Parameters (in Angstroms) for Intermediates Involved in MSR on $Pt_3Sn(111)$.

Species	**Site**[a]	**Mode**	$d_{C/O\text{-}Pt/Sn}$	E_{ads}
CH_2OOH	B^{2Pt}	$\eta^1(O)$-$\eta^1(O)$	2.14, 2.35	1.65
	B^{PtSn}	$\eta^1(O)$-$\eta^1(O)$	2.15, 2.31	1.89
CH_2OO	B^{PtSn}	$\eta^1(O)$-$\eta^1(O)$	2.05, 2.07	3.08
	F^{2PtSn}	$\eta^2(O)$-$\eta^1(O)$	2.09, 2.26, 2.27	3.24
HCOOH	T^{Pt}-V^b	$\eta^1(O)$	2.41	0.38
	T^{Sn}-V^b	$\eta^1(O)$	2.58	0.49
	F^{2PtSn}-P^b			0.41
	F^{3Pt}-P^b			0.36
	H^{2PtSn}-P^b			0.39
	H^{3Pt}-P^b			0.37
CHOO	B^{2Pt}	$\eta^1(O)$-$\eta^1(O)$	2.20, 2.20	2.28
	B^{PtSn}	$\eta^1(O)$-$\eta^1(O)$	2.17, 2.29	2.52
COOH-*cis*	T^{Pt}	$\eta^1(C)$	2.03	2.48
	T^{Sn}	$\eta^1(C)$	2.32	1.26
	B^{2Pt}	$\eta^1(C)$-$\eta^1(O)$	2.01, 2.36	2.37
COOH-*trans*	T^{Pt}	$\eta^1(C)$	2.06	2.35
	T^{Sn}	$\eta^1(C)$	2.34	1.09
	B^{2Pt}	$\eta^1(C)$-$\eta^1(O)$	2.02, 2.37	2.39
	B^{PtSn}	$\eta^1(C)$-$\eta^1(O)$	2.04, 2.55	2.41
CO_2	B^{2Pt}			0.11
	B^{PtSn}			0.11
H_2O	T^{Pt}			0.01
	T^{Sn}			0.01
OH	T^{Pt}	$\eta^1(O)$	2.04	2.34
	T^{Sn}	$\eta^1(O)$	2.04	2.50
	B^{2Pt}	$\eta^2(O)$	2.23, 2.24	2.51
	B^{PtSn}	$\eta^2(O)$	2.25, 2.27	2.49

[a] V and P represent the O–H axis almost vertical and parallel to the surface.