Supplementary Information

Role of Sn promoter in Ni/Al_2O_3 catalyst for the deoxygenation of stearic acid and coke formation: experimental and theoretical studies

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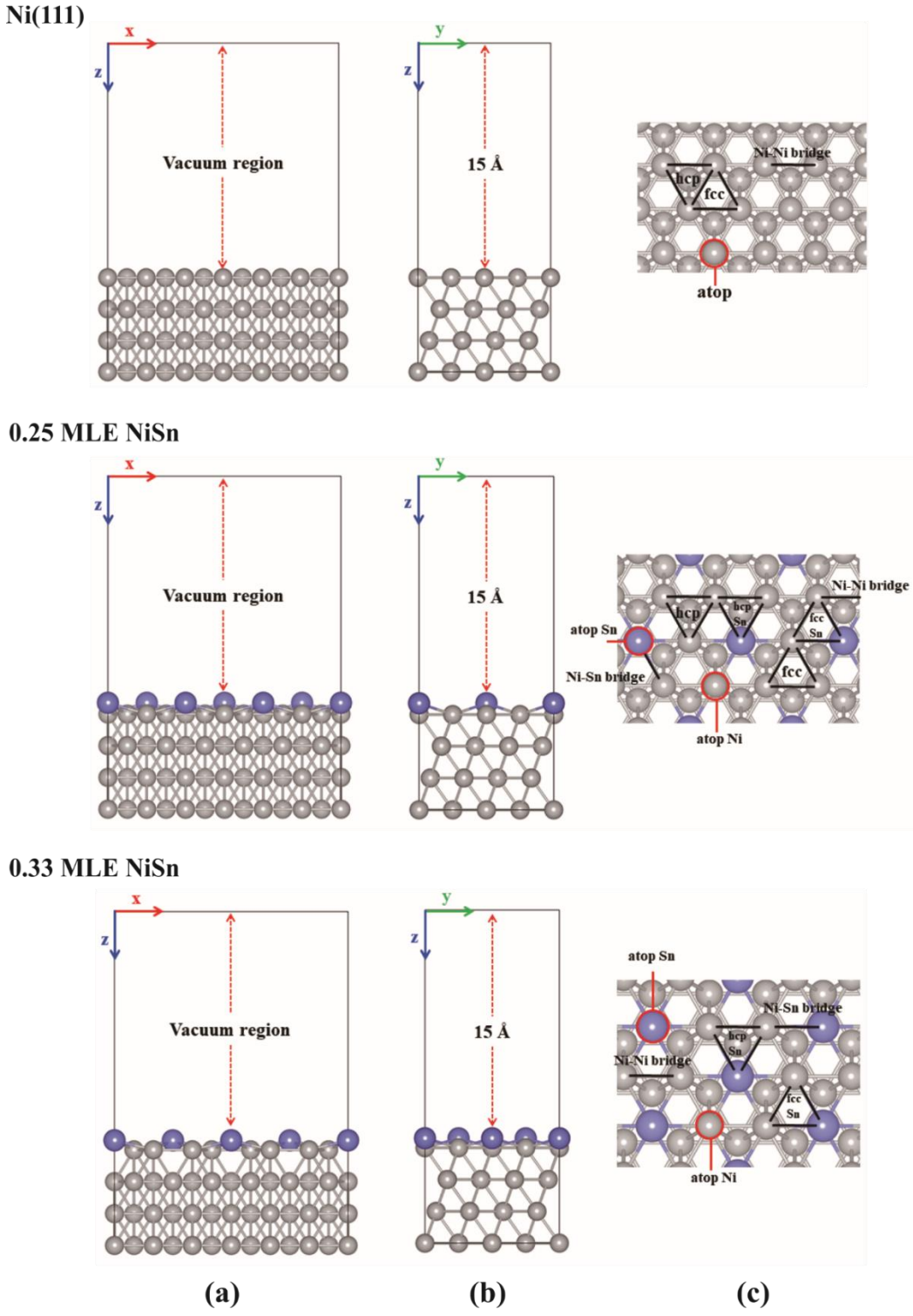

Fig. S1. Surface slab structures of (a) bare Ni(111), (b) 0.25 MLE NiSn surface and (c) 0.33 MLE NiSn surface. The models are projected along the (010)-direction (left), (100)-direction (middle). The possible active sites of each surface are presented in the right panel.

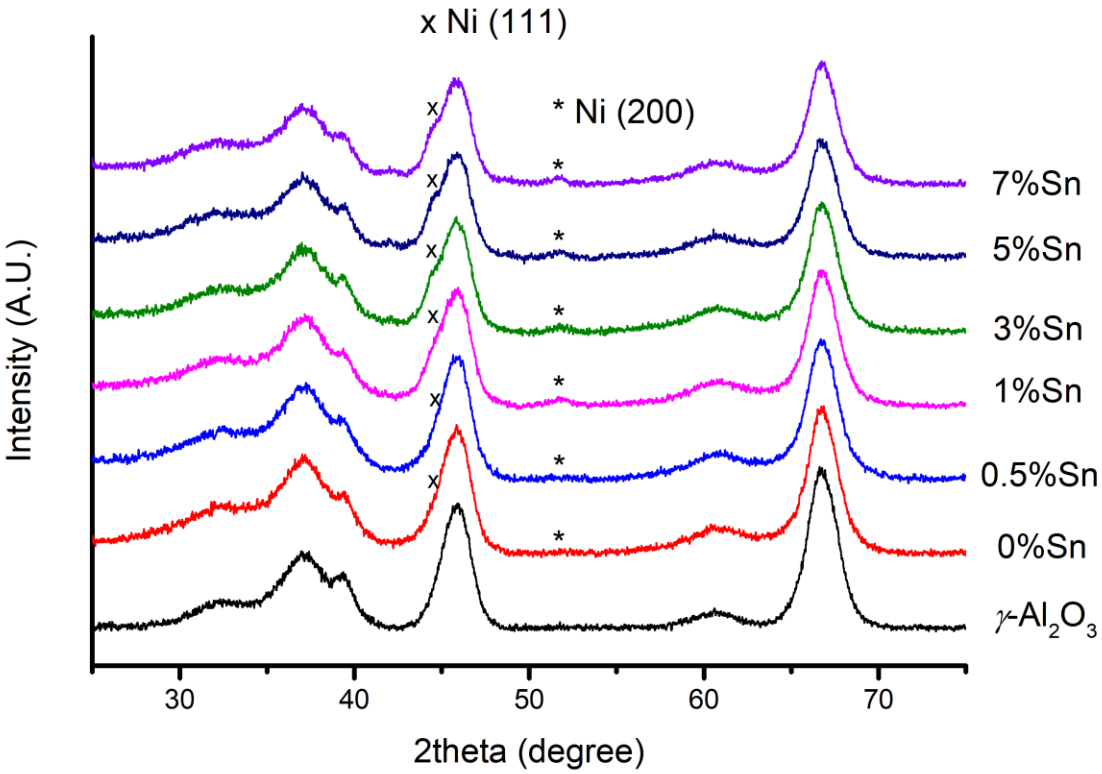

Fig. S2. XRD patterns of NiSn/γ-Al_2O_3 catalysts containing 18 wt% Ni and various Sn loading (wt%).

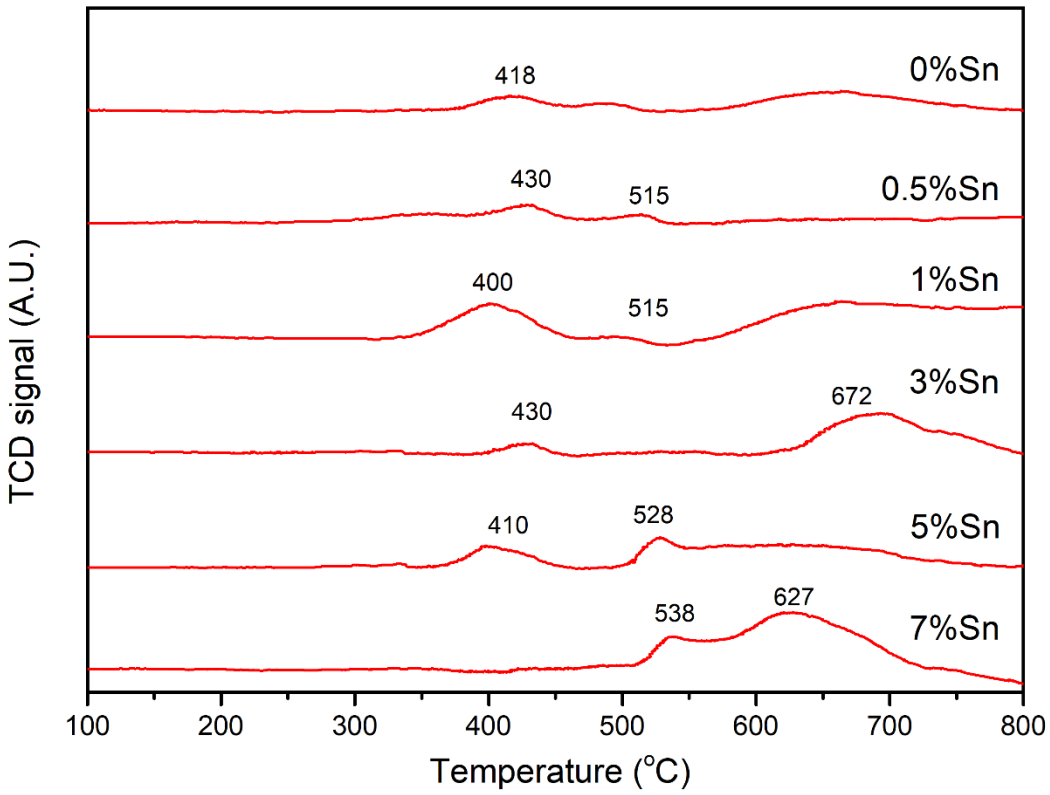

Fig. S3. H_2-TPR profiles of NiSn/γ-Al_2O_3 catalysts containing 18 wt% Ni and various Sn loading.

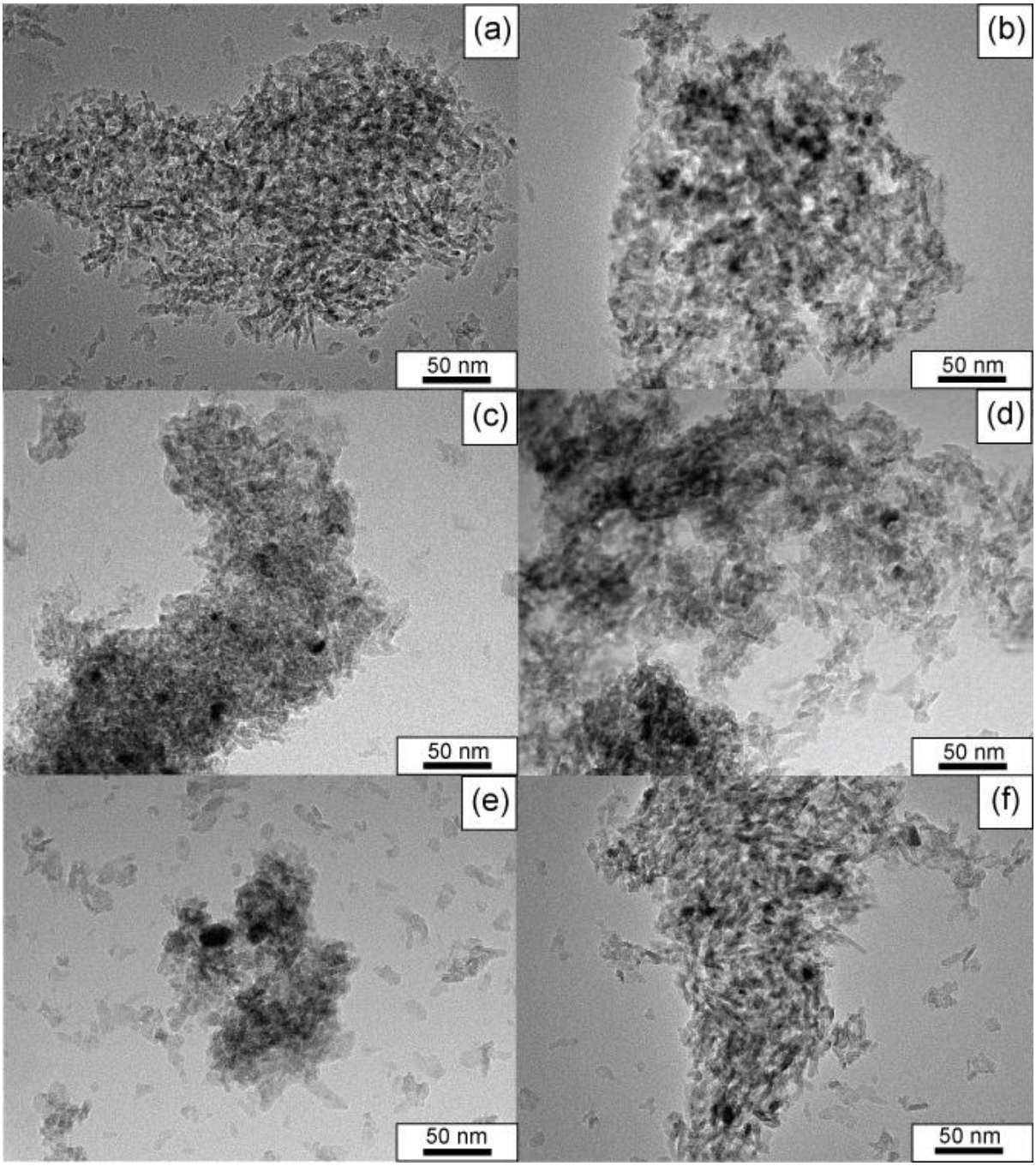

Fig. S4. TEM images of NiSn/γ-Al_2O_3 catalysts containing 18 wt% Ni and various Sn loading: (a) 0 wt% Sn, (b) 0.5 wt% Sn, (c) 1wt% Sn, (d) 3 wt% Sn, (e) 5 wt% Sn, and (f) 7 wt% Sn.

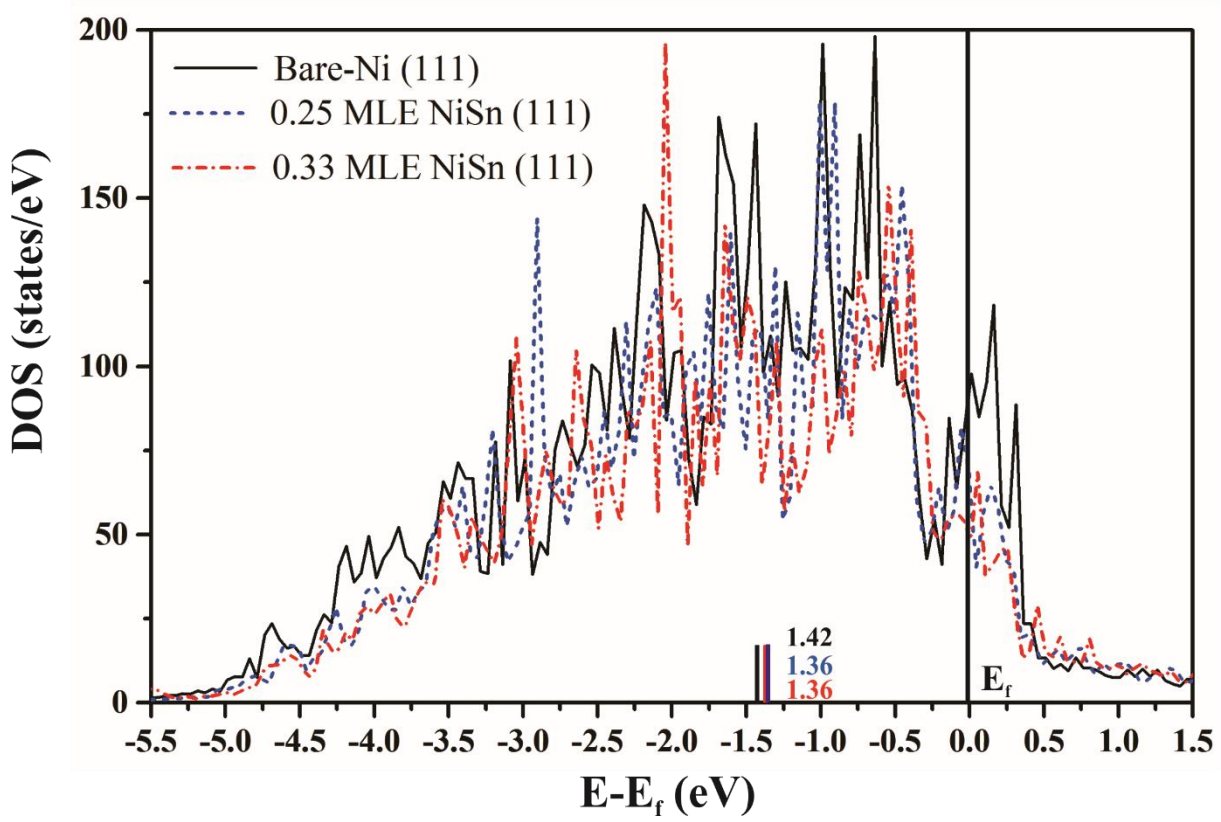

Fig. S5. The projected density of states (PDOS) of bare Ni(111), 0.25 MLE and 0.33 MLE of NiSn surfaces.

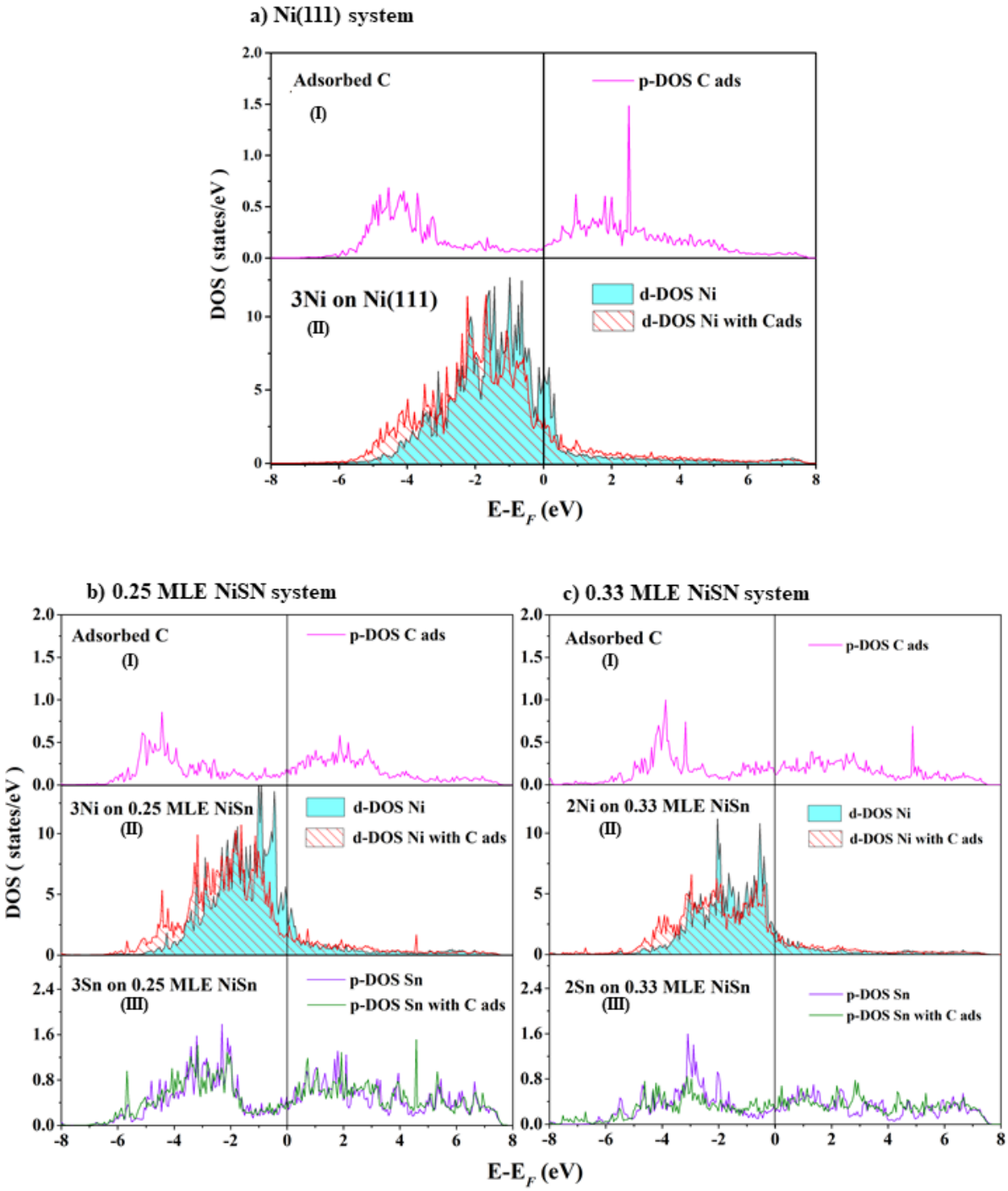

Fig. S6. Comparison projected density of states (PDOS) of selected atoms in the C adsorption on (a) Ni(111), (b) 0.25 MLE NiSn and (c) 0.33 MLE NiSn systems. Panel I illustrates p-DOS of the adsorbed C atom. Panel II presents d-DOS of Ni atom of substrates before and during C adsorption. Panel III depicts p-DOS of Sn on 0.25 and 0.33 MLE of NiSn surfaces before and during C adsorption.

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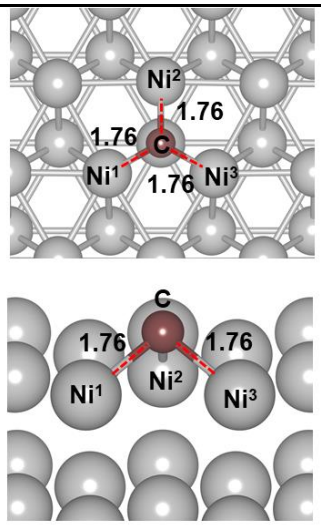
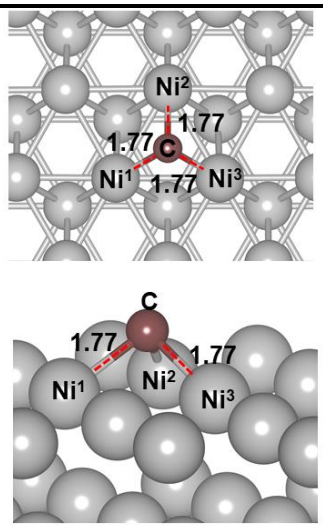
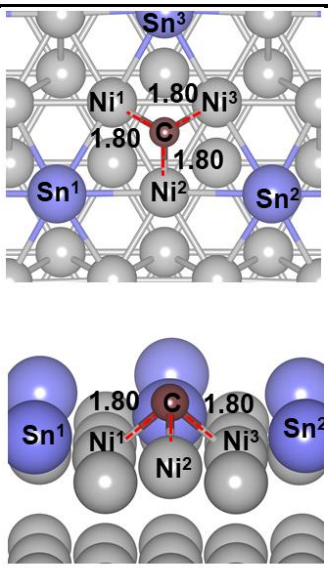
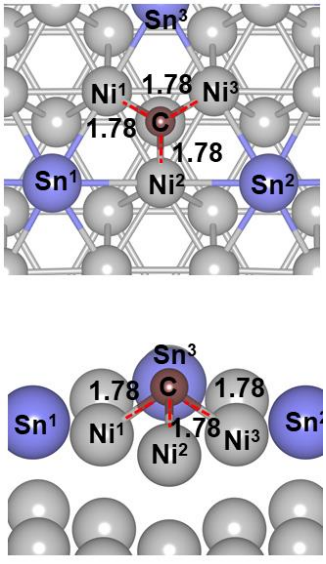
Table S1 Atomic ratio of Ni and Sn species in NiSn/γ-Al_2O_3 catalysts obtained from XPS spectra.

Catalysts	Atomic ratio	
	Ni^0/Ni^{2+}	Sn^0/Sn^{2+}
18 wt% Ni/γ-Al_2O_3	0.77	n/a
1 wt% Sn 18 wt% Ni/γ-Al_2O_3	0.63	0.57
3 wt% Sn 18 wt% Ni/γ-Al_2O_3	0.82	0.83
5 wt% Sn 18 wt% Ni/γ-Al_2O_3	2.12	0.61
7 wt% Sn 18 wt% Ni/γ-Al_2O_3	1.78	1.10

Table S2. All possible adsorption configuration of C atom on Ni(111), 0.25 MLE and 0.33 MLE NiSn surfaces.

Surface	Geometry	Favored site	E_{ads} (eV)
Pristine Ni(111)		hcp	-6.99
		fcc	-6.95

Surface	Geometry	Favored site	E_{ads} (eV)
0.25 MLE NiSn		fcc	-6.24
		hcp	-6.24

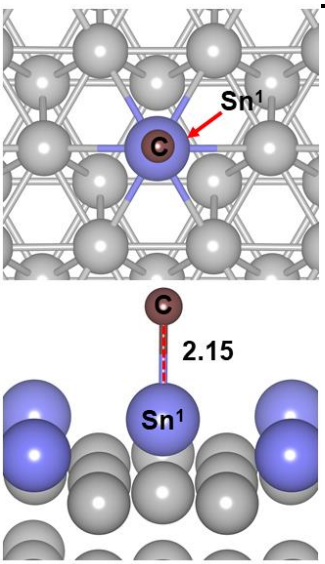
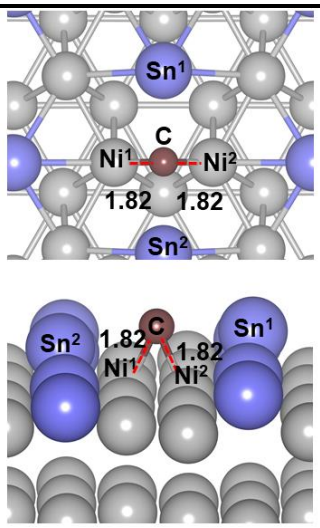
Surface	Geometry	Favored site	E_{ads} (eV)
		atop Sn	-1.98
0.33 MLE NiSn		Ni-Ni Bridge	-5.12

Table S3. The d-band center (ε_d) of the nearest Ni atom of the adsorbed C atom on Ni(111), 0.25 and 0.33 MLE of NiSn surface.

Surface	ε_d (eV)	
	Before C adsorption	During C adsorption
Ni(111)	-1.27	-1.54
0.25MLE NiSn	-1.21	-1.68
0.33MLE NiSn	-1.25	-1.74