Supplementary Material

Insight into the electronic modulation of bimetallic Pt-Sn cluster for selective hydrogenation of 1,3-butadiene

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Table S1. Elemental composition of PtSn catalysts determined by ICP-OES.

Catalysts	Pt wt.%	Sn wt.%	K wt.%	Sn/Pt atomic ratio	CO uptake (mol/gcat)
PtSn1/S-1	0.36	0.22	0.44	1.00	5.57
PtSn3/S-1	0.35	0.64	0.43	3.01	5.11
PtSn10/S-1	0.34	2.07	0.41	10.01	2.40

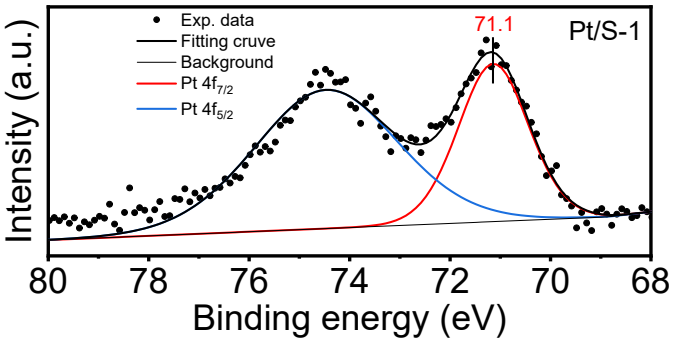

Fig. S1. Pt 4f spectra of reduced Pt/S-1 samples. The sample were reduced by H_2 at 600°C for 1 h prior to XPS measurement.

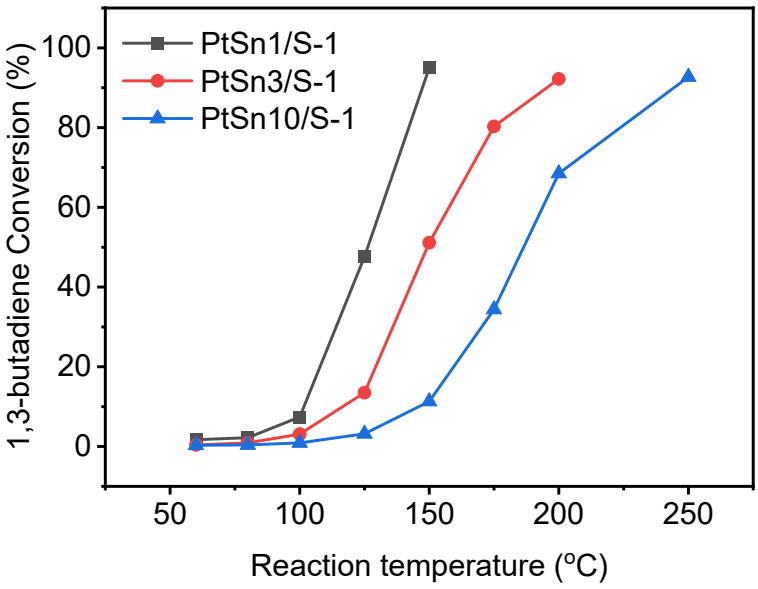

Fig. S2 The 1,3-butadiene conversion as a function of reaction temperature over different samples.

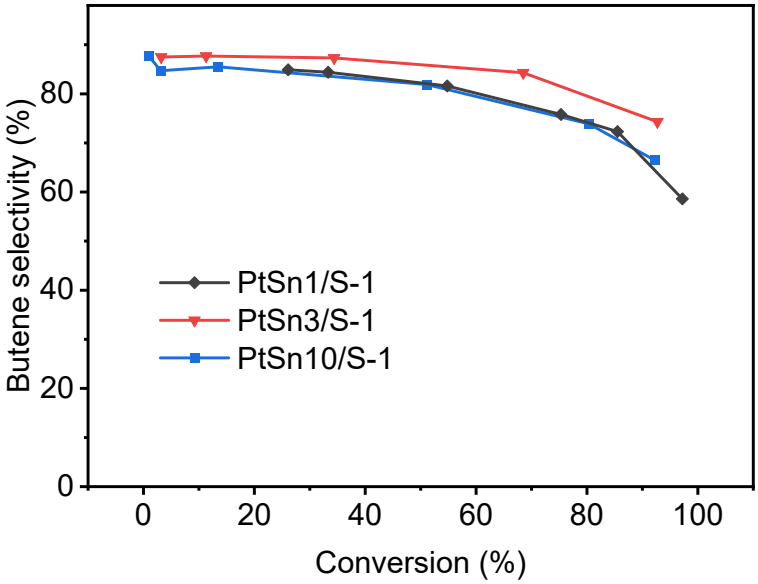

Fig. S3 The butene selectivity as a function of 1,3-butadiene conversion over PtSn/S-1 samples.

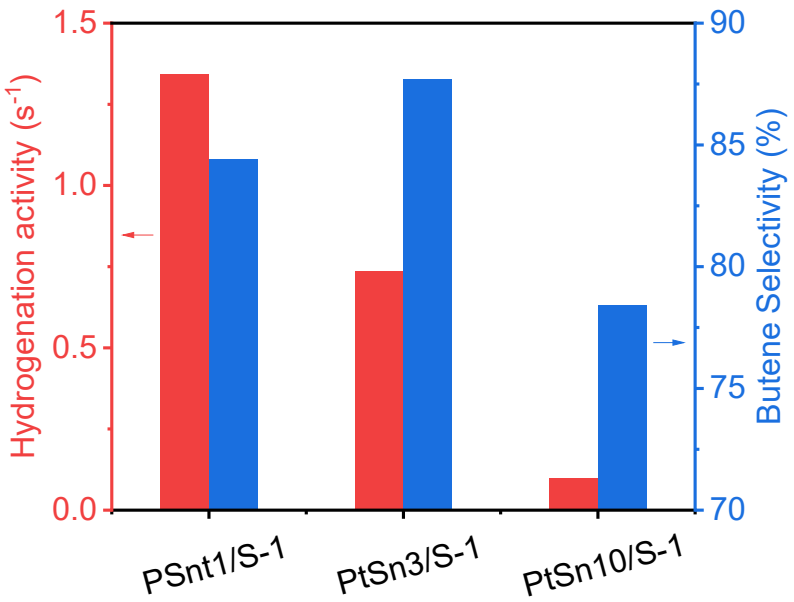

Fig. S4. Initial specific activity and butene selectivity of the PtSn/S-1 samples during hydrogenation of 1,3-butadiene in the absence of CO. All the samples were reduced by H_2 at 600 °C for 3h prior to catalytic evaluation. Reaction condition: 10 mg samples, 125 °C, 4 ml/min H_2, 20 ml/min 2%1,3-butadiene/N_2.

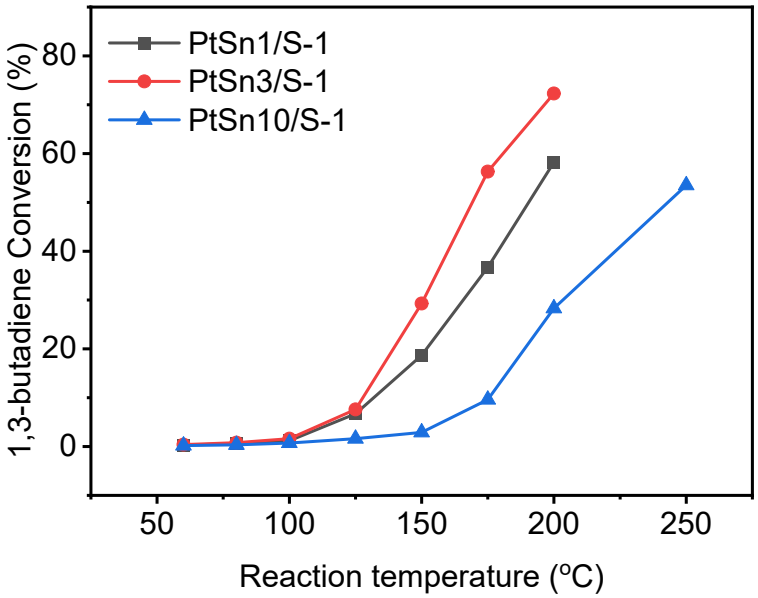

Fig. S5 The 1,3-butadiene conversion as a function of reaction temperature over different samples in the presence of CO.

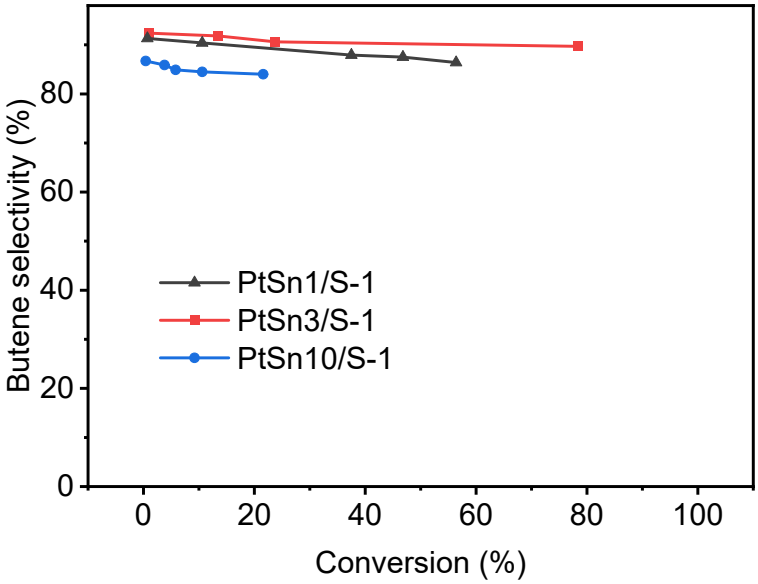

Fig. S6 The butene selectivity as a function of reaction temperature over different samples in the presence of CO.

Table S2. Catalytic performance for different PtSn catalysts in the 1,3-butadiene hydrogenation at 125°C. Data were acquired under the kinetic region with conversion <40% by tuning the space velocity.

Catalysts	TOF (s^{-1})[a]	TOF (s^{-1})[b]	Selectivity (%)				Butene sel. (%)
			1-butene	*cis*-2-butene	*trans*-2-butene	butane	
PtSn1/S-1	1.34	4.45	55.6	11.9	16.9	15.6	84.4
PtSn3/S-1	0.74	2.58	58.0	11.8	17.9	12.3	87.7
PtSn10/S-1	0.10	0.71	49.8	11.7	16.9	21.6	78.4

[a] TOF is determined by the overall content of Pt in the catalysts.
[b] TOF is determined by CO uptake.

Table S3. Catalytic performance for different PtSn catalysts among the 1,3-butadiene hydrogenation at 125°C in the presence of CO. Data was acquired under the kinetic region with conversion <40% by tuning the space velocity.

Catalysts	TOF	Selectivity (%)				Butene sel. (%)
	$(h^{-1})^a$	1-butene	*cis*-2-butene	*trans*-2-butene	butane	
PtSn1/S-1	0.36	56.0	12.4	19.5	12.1	87.9
PtSn3/S-1	0.41	54.3	14.9	23.2	7.6	92.4
PtSn10/S-1	0.08	54.1	12.5	18.8	14.5	85.5

[a] TOF is determined by the overall content of Pt in the catalysts.

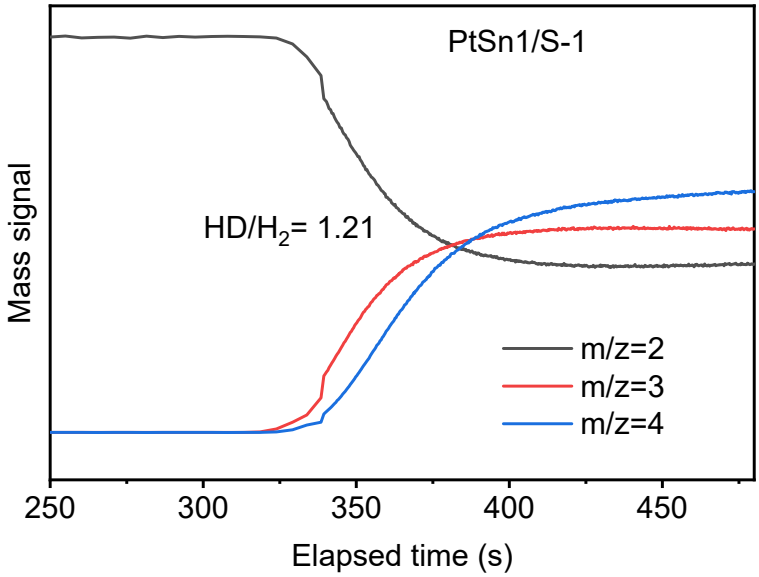

Fig. S7 H_2-D_2 exchange profile of PtSn1/S-1 samples after reduction in H_2 at 600 °C for 3 h.

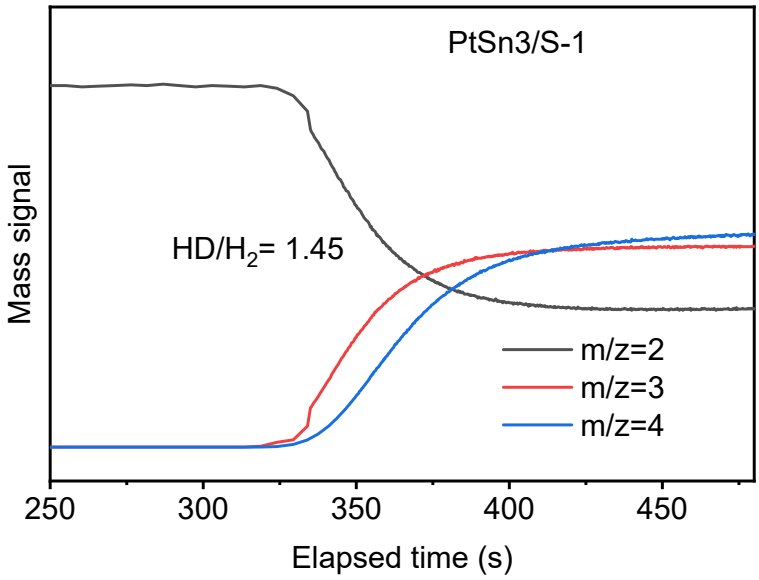

Fig. S8 H_2-D_2 exchange profile of PtSn3/S-1 samples after reduction in H_2 at 600 °C for 3 h.

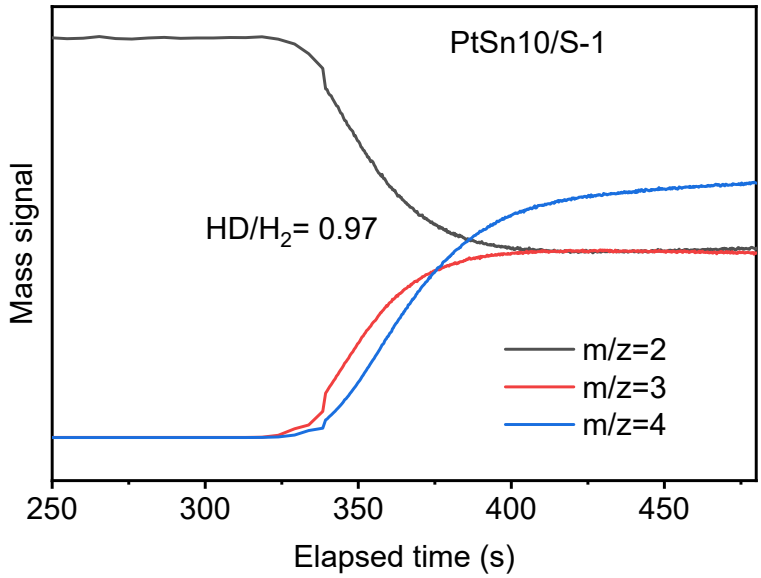

Fig. S9 H_2-D_2 exchange profile of PtSn10/S-1 samples after reduction in H_2 at 600 °C for 3 h.

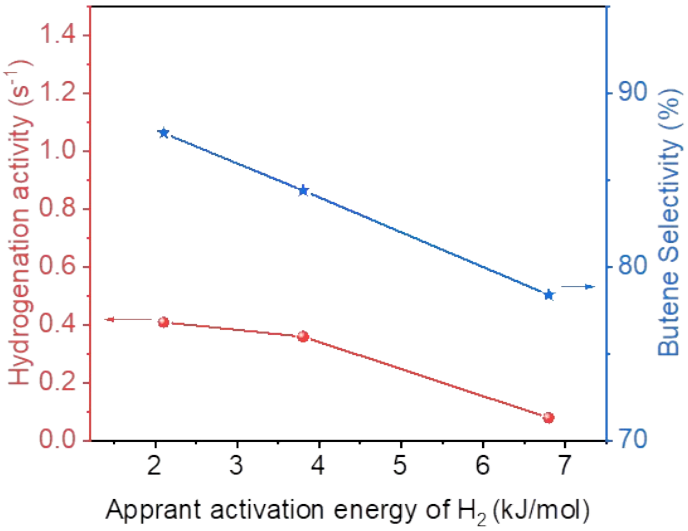

Fig. S10. Proposed correlation between the energy barrier of H_2 dissociation and intrinsic hydrogenation of activity and butene selectivity.