Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Reaction induced robust Pd_XBi_Y/SiC catalyst for the gas phase oxidation of monopolistic alcohols

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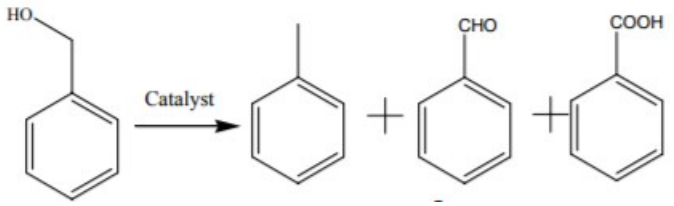
The calculation method of benzyl alcohol conversion and benzaldehyde selectivity



Correction factor: $$fi = \frac{m_i}{m_D} * \frac{A_D}{A_i}$$

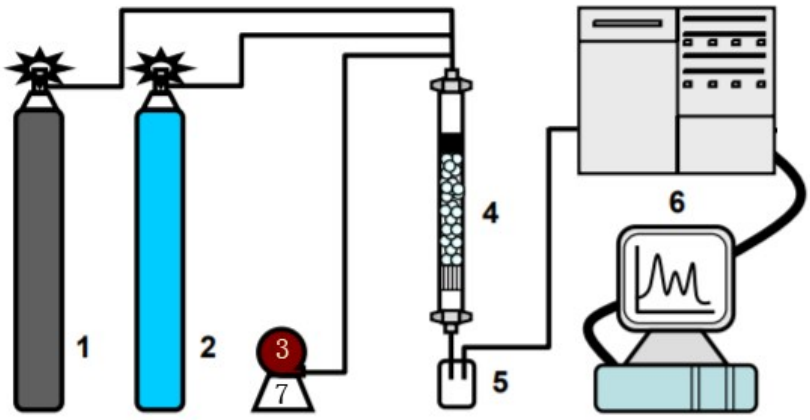
m_i: the weight of the substance; m_D: the weight of internal material DMSO; A_D: the peak area of DMSO in gas chromatography (GC); A_i: the peak area of the substances in GC.

benzyl alcohol conversion: $$Conver. = 1 - \frac{m_D^{'} * f_P * \frac{A_P^{'}}{A_D^{'}}}{m_P}$$

$m_D^{'}$: the weight of DMSO added into the system; f_P: correction factor of benzyl alcohol; $A_P^{'}$: the peak area of benzyl alcohol after reaction; $A_D^{'}$: the peak area of DMSO added into the system; m_P: the weight of benzyl alcohol added before the reaction

Benzyl aldehyde selectivity: $$Sel. = \frac{m_D^{'} * f_t * \frac{A_t}{A_D^{'}}}{m_P * Conver.}$$

f_t: correction factor of benzaldehyde; A_t: the peak area of benzaldehyde after reaction



Scheme S1. The fix-bed reactor used in alcohol oxidation

(1. N_2 cylinder; 2. O_2 cylinder; 3. Pump; 4. Reactor tube; 5. Condensator; 6. GC; 7. alcohol)

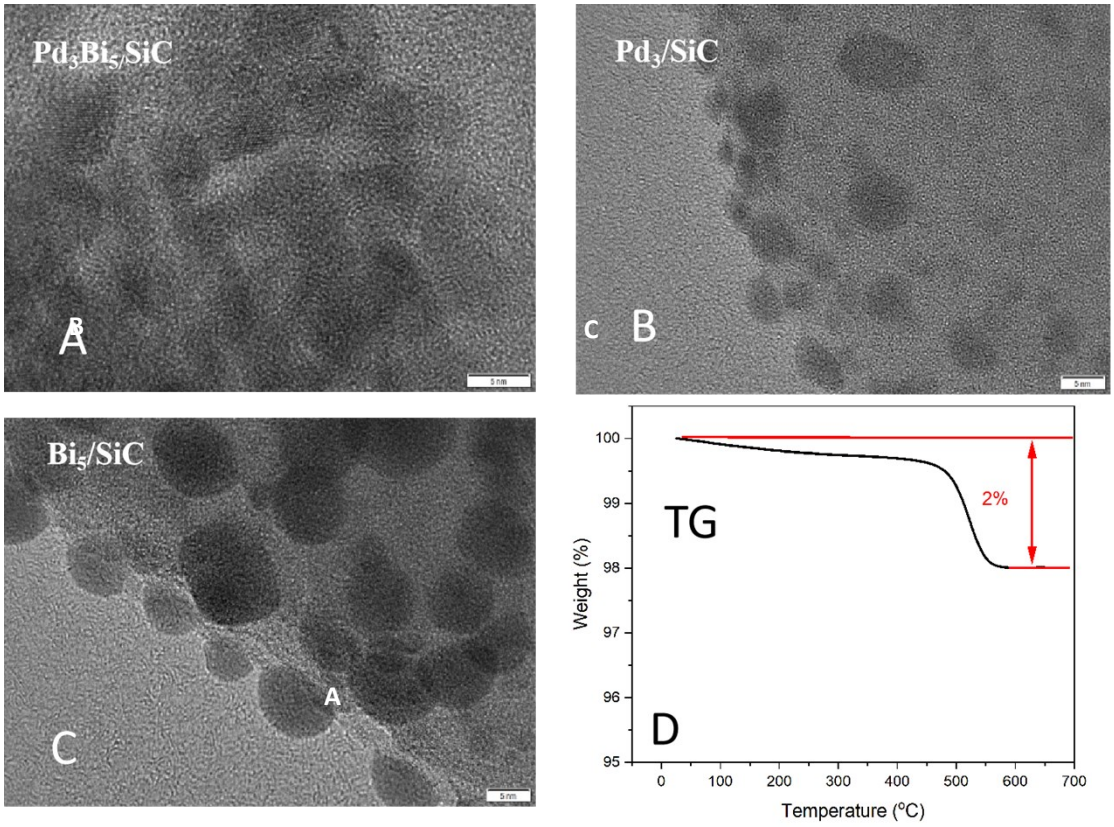


Fig. S1. TEM images of Pd_3Bi_5/SiC fresh (A), used Pd_3/SiC (B), used Bi_5/SiC catalysts (C) and TG curve of used Pd_3Bi_5/SiC (D)

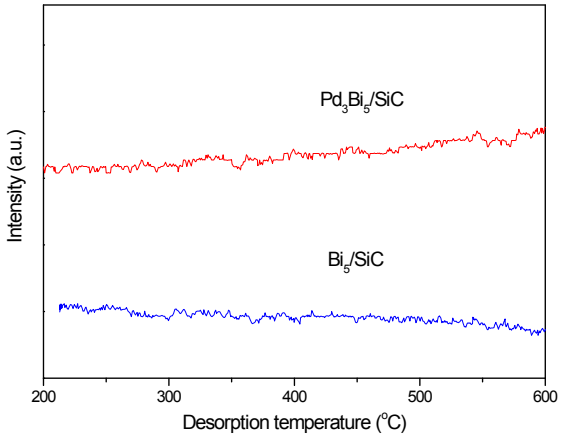


Fig. S2. O_2-TPD profiles of the catalysts

Table S1. Catalytic performance of Pd_3Bi_5/SiC

Alcohol	Temperature (°C)	Conversion (%)	Selectivity (%)
1-phenylethanol	280	75	98
2-phenylethanol	300	55	97
methanol	280	91	92
ethanol	290	88	93

Table S2. The turnover frequencies (TOFs) of benzyl alcohol oxidation over the catalysts based on Pd NPs[a].

Catalyst	V_{total}[b] ($\times 10^{-4}$, cm^3)	D_{Pd}[c] (nm)	$V_{Pd\text{-}particle}$[d] (nm^3)	Amount of Pd Particles ($\times 10^{14}$)	$S_{Pd\text{-}particle}$[e] (nm^2)	S_{total} (cm^2)	Amount of Surface Ag Atoms[e] ($\times 10^{18}$)	Conv.[f] (%)	N[g] ($\times 10^{22}$)	TOF (h^{-1})
Pd_3Bi_5/SiC[h]	7.5	5.8	51	147	52.8	7761	11.4	12	10.08	8842
Pd_3Bi_5/SiC[i]	7.5	5.8	51	147	52.8	7761	11.4	3	2.52	2210
Pd_3/SiC[h]	7.5	5.5	43	174	47.5	8265	12.2	0.3	0.252	206
Pd_3/SiC[i]	7.5	5.5	43	174	47.5	8265	12.2	0.1	0.080	65

[a]For each catalyst, 0.3 g was used in testing experiments; [b]The total volume of Pd (V_{total}) is calculated as: Pd mass (0.3 g × Pd-loading (wt%)) is divided by the silver density (12 g/cm^3); [c]The particle size is estimated from TEM images; [d]The Pd NPs are assumed as hemisphere, and the volume of single Pd particle is $\pi D_{Pd}^3/12$, and the surface area is $\pi D_{Pd}^2/2$; [e]The distance between the adjacent Pd atoms is 0.26 nm, and one Pd atom occupies the surface area of 0.0676 (0.26 × 0.26 = 0.0676) nm^2; [f]The weight hourly space velocity (WHSV) = 500 h^{-1}, and 150 g benzyl alcohol was fed into the reactor; [g]Amount of converted benzyl alcohol (Take the converted benzyl alcohol over the catalyst Pd_3Bi_5/SiC as example: the converted benzyl alcohol in one hour is 18 g (150 × 0.12 = 18 g), and the converted amount of benzyl alcohol molecule is 3.36×10^{22} (18 (g) ÷ 108 (g/mol) = 0.1668 mol; $0.1668 \times 6.02 \times 10^{23} = 10.08 \times 10^{22}$)); [h]260 °C; [i]240 °C.