

Direct C–C coupling of bio-ethanol into 2,3-butanediol by photochemical and photocatalytic oxidation with Hydrogen peroxide

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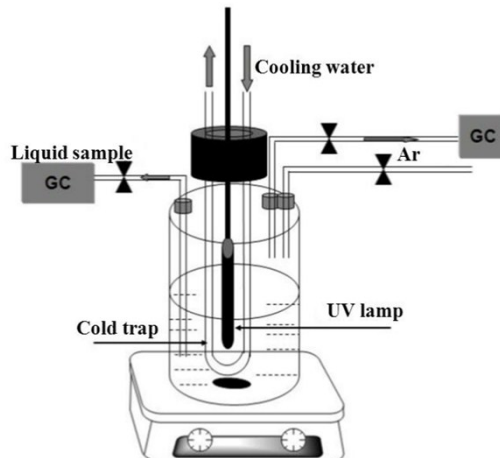
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Supplementary Information

This Supplementary Information contains Figures S1-S3 and Table S1-S2.



Figures S1: A schematic of the employed photochemical and photocatalytic reactor

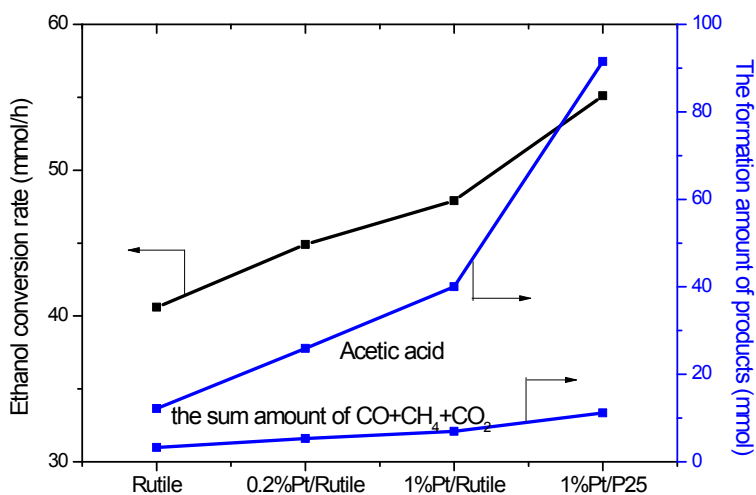


Figure S2 the formation amount of by-product and ethanol conversion rate as a function of different photocatalysts. Reaction reaction: 298K, ethanol 0.959mol, aqueous solution H₂O₂ (30%) (0.1mol) was added by successive addition at 2ml/h for 5h, 0.2g of catalyst, with 0.2% or 1% of Pt co-catalyst 200 ml; 300 W high pressure Hg lamp.

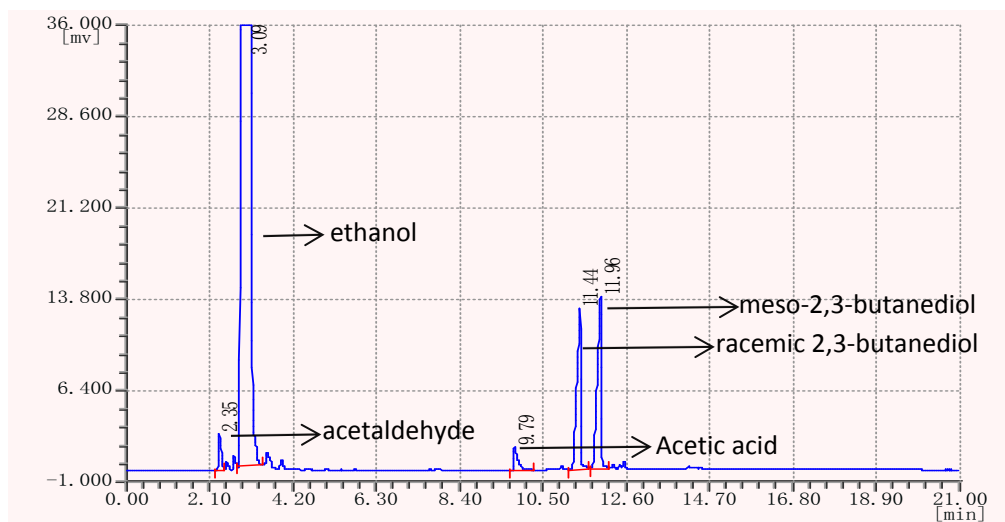


Figure S3: Gas chromatogram of the liquid products obtained under UV irradiation (Reaction conduction: 298K, ethanol 0.959mol, aqueous solution H₂O₂ (30%) 0.1mol, 200 ml); We employed a gas chromatograph to analyze the Liquid samples which was confirmed by comparing the mass spectrum and retention of standard pure sample. The products name was mark in the chromatogram. The 2,3-BDO included racemic-2,3-BDO and meso-2,3-BDO.

Table S1. Experimental data for the photocatalytic C-C coupling of ethanol^a

$$\text{CH}_3\text{CH}_2\text{OH} + \text{H}_2\text{O}_2 \xrightarrow{h\nu} \text{CH}_3\text{CH}(\text{OH})\text{CH}(\text{OH})\text{CH}_3 + \text{H}_2\text{O}$$

Entry	catalyst	Con. (%)	Selectivity (%)			Gas formation rate ^b of (CO+CH ₄ +CO ₂) (μmol h ⁻¹)	Formation rate of 2,3-BDO ^c (mmol h ⁻¹)
			2,3-BDO	Aldehyde	Acetic acid		
1	no	19.4	91.3	2.14	1.90	546	15.3
2	Rutile	22.4	86.1	1.06	6.03	654	17.5
3	0.2%Pt/Rutile	24.9	81.4	1.65	11.3	1064	18.3
4	1%Pt/Rutile	26.8	61.9	1.83	16.7	1394	14.9
5	1%Pt/P25	31.4	36.5	1.54	33.2	2240	10.1
6	SiO ₂	25.0	75.5	1.73	4.18	818	16.0
7	SBA-15	27.9	72.5	1.79	5.68	1046	18.0
8	γ-Al ₂ O ₃	32.1	68.6	1.35	5.96	1194	18.9

^a Reaction condition: 298K, ethanol 0.959mol, aqueous solution H₂O₂ (30%) 0.1mol was added by successive addition at 2ml/h, 0.2g of catalyst with 0.2% or 1% of Pt co-catalyst, 200 ml; 300 W high pressure Hg lamp (λ=365 nm), 5h of irradiation time. ^b The rate was calculated on the basis sum of the CO, CH₄ and CO₂ formation rate; ^c The rate was calculated on the basis of the generated 2,3-BDO.

Table S2. The repeatability of photochemical reaction

Entry	Conversion (%)	Selectivity (%)		
		2,3-BDO	Aldehyde	Acetic acid
1	19.4	91.3	2.14	1.90
2	18.5	92.3	1.21	1.30
3	20.1	90.5	3.21	2.10

Reaction conduction: 298K, ethanol 0.959mol, aqueous H₂O₂ (30%) 0.1mol was added by successive addition at 2ml/h for 5h, 200 ml; 300 W high pressure Hg lamp (λ=365 nm); The conversion of ethanol and the 2,3-BDO selectivity had negligible changes for three repeated experiments, confirming good repeatability for this method.