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Electronic Supplementary Information (ESI) Bifunctional heterogeneous catalysts derived from the coordination of adenosine monophosphate to Sn(IV) for effective conversion of sucrose to 5-hydroxymethylfurfural

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Scheme S1. Molecular structure of adenosine monophosphate.



Figure S1. SEM image of AMP.

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Figure S2. Pore size distribution of Sn-AMP_{0.5}.

Figure S3 shows the Raman spectra for fresh Sn-AMP_{0.5} and Sn-AMP_{0.5} after interacting with glucose (Sn-AMP_{0.5}+glucose) and with fructose (Sn-AMP_{0.5}+fructose). The peaks at 1318 and 1424 cm⁻¹ are attributed to the adenine ring breathing mode.^{S1,S2} The peaks at 1340 and 1404 cm⁻¹ are attributed to the sugar stretching mode.^{S1,S2} The interactions of glucose and fructose with Sn-AMP_{0.5} resulted in the intensity changes of these peaks. The peaks at 965 and 1015 cm⁻¹ of fresh Sn-AMP_{0.5}+glucose and Sn-AMP_{0.5}+fructose, attributed the interactions of glucose and fructose with the phosphate and N1 of AMP. The Raman spectra can prove the hydrogen bonding interactions of glucose and fructose with Sn-AMP_{0.5}.



Figure S3. Raman spectra in the region of 900-1800 cm⁻¹ for fresh Sn-AMP_{0.50} (black), Sn-AMP_{0.5} after interacting with glucose (blue), and Sn-AMP_{0.5} after interacting with fructose (oliver).

Raman spectra were recorded using a Raman microscope (Kaiser Optical Systems, Inc., Ann Arbor, MI, USA) with 785 nm laser excitation.

	AMP (cm ⁻¹)	Sn-AMP (cm ⁻¹)
NH ₂ - scissor mode	1695	1695
NH ₂ - bending mode	1650	1650
C4-C5 skeletal vibrations	1595	—
pyrimidine ring vibration	1557	1548
imidazole	1504	1514
N7-C8	1463	1463
C6-N1	1421	1421
pyrimidine	1385	1407
C6-NH ₂ deformation	1280	
	1198	
ribose C-O stretching vibration	1102	
	1036	
P-O-H vibration	1062,985	

Table S1. FTIR spectra data of AMP and Sn-AMP_{0.5}.

Table S2	. During the s	ynthesis proc	cess for the	Sn-AMP s	samples, th	ne pH of the	e solutions a	after
hydrothe	rmal treatmen	t.						

	Sn-AMP _{0.125}	Sn-AMP _{0.25}	Sn-AMP _{0.5}	Sn-AMP _{0.75}
pН	1.29	1.34	1.40	1.56

Table S3. Comparison of catalytic activity of Sn-AMP catalysts for dehydration of glucose.

Entry	Catalyst	X (%)	Y_{HMF} (%)	$Y_{fructose}$ (%)	Y_{FA} (%)
1	Sn-AMP _{0.125}	95.7	54.0	4.2	1.8
2	Sn-AMP _{0.25}	96.8	62.1	5.0	2.1
3	Sn-AMP _{0.5}	96.4	63.5	4.1	2.0
4	Sn-AMP _{0.75}	97.1	56.4	3.1	2.2

Reaction condition: glucose (200 mg), Sn-AMP (50 mg), 5 mL of solvent, water/THF (v:v 1:4), 160 °C, 5h.

Table S4. Comparison of Sn-AMP with other ca	alysts. (Yield: HMF yield, Sel.: HMF selectivity)

saccharide	Solvent	Catalyst	T/°C	t/h	Yield	Sel.	Ref.
ucrose			170	4	61.6%	≥64.8%	
glucose	water/DMSO/HCL	Sn-CP	170	4	63.9%	65.4%	S3
sucrose	water/THE/NaCl	Sn Mont	160	2	43.6%	-	S4
glucose	water/Inr/NaCi	Sn-Mont	100	3	41.7%	-	
sucrose	watar/Diavara	$S_{\rm m} R/A_{\rm m}$ have barries 121	00	10	60.0%	-	S 5
glucose	water/Dioxane	Sn-p/Amberlyst-151	90	16	56.0%	-	33
sucrose		Phosphated TiO ₂	175	2	43.0%	45.3%	\$6
glucose	water/1111/1NaCI			4	53.5%	54.3%	30
sucrose	water /GVI /NaCl	APG-SO ₃ H	180	4	56.2%	-	S7
glucose	water /OvL/Maci				52.9%	-	
sucrose	water/THE	[MimAM]nH3-nPW ₁₂ O ₄₀	160	7.5	23.5%	24.9%	<u>c</u> e
glucose	water/1m				39.2%	39.5%	30
sucrose	water/THF	Sn-AMP _{0.5}	160	4.5	62.9%	63.0%	This
glucose	water/THF		160	5	67.5%	69.6%	work

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