## Electronic Supplementary Information (ESI)

## Bifunctional heterogeneous catalysts derived from the coordination of adenosine monophosphate to $\mathrm{Sn}(\mathrm{IV})$ for effective conversion of

 sucrose to 5-hydroxymethylfurfuralChenyu Wang, Lutong Jiao, Han Meng, Peijun Ji ${ }^{*}$

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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 $\mathrm{Sn}-\mathrm{AMP}_{0.5}$.
Figure S 3 shows the Raman spectra for fresh $\mathrm{Sn}-\mathrm{AMP}_{0.5}$ and $\mathrm{Sn}-\mathrm{AMP}_{0.5}$ after interacting with glucose ( $\mathrm{Sn}-\mathrm{AMP}_{0.5}+$ glucose) and with fructose $\left(\mathrm{Sn}-\mathrm{AMP}_{0.5}+\right.$ fructose). The peaks at 1318 and $1424 \mathrm{~cm}^{-1}$ are attributed to the adenine ring breathing mode. ${ }^{\mathrm{S} 1, \mathrm{~S} 2}$ The peaks at 1340 and 1404 $\mathrm{cm}^{-1}$ are attributed to the sugar stretching mode. ${ }^{\mathrm{S1}, \mathrm{~S} 2}$ The interactions of glucose and fructose with $\mathrm{Sn}-\mathrm{AMP}_{0.5}$ resulted in the intensity changes of these peaks. The peaks at 965 and 1015 $\mathrm{cm}^{-1}$ of fresh $\mathrm{Sn}-\mathrm{AMP}_{0.5}$ are attributed to $\mathrm{OH}-\mathrm{P}$ and N1-C6. ${ }^{\mathrm{S1}, \mathrm{~S} 2}$ These peaks did not appear in the spectra of $\mathrm{Sn}-\mathrm{AMP}_{0.5}+$ glucose and $\mathrm{Sn}-\mathrm{AMP}_{0.5}+$ 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 $\mathrm{Sn}-\mathrm{AMP}_{0.5}$.


Figure S3. Raman spectra in the region of $900-1800 \mathrm{~cm}^{-1}$ for fresh $\mathrm{Sn}-\mathrm{AMP}_{0.50}$ (black), $\mathrm{Sn}-\mathrm{AMP}_{0.5}$ after interacting with glucose (blue), and $\mathrm{Sn}-\mathrm{AMP}_{0.5}$ 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.

Table S1. FTIR spectra data of AMP and $\mathrm{Sn}-\mathrm{AMP}_{0.5}$.

|  | AMP $\left(\mathrm{cm}^{-1}\right)$ | Sn-AMP $\left(\mathrm{cm}^{-1}\right)$ |
| :--- | :--- | :--- |
| $\mathrm{NH}_{2}$ - scissor mode | 1695 | 1695 |
| $\mathrm{NH}_{2}$ - bending mode | 1650 | 1650 |
| C4-C5 skeletal vibrations | 1595 | - |
| pyrimidine ring vibration | 1557 | 1548 |
| imidazole | 1504 | 1514 |
| $\mathrm{~N} 7-\mathrm{C} 8$ | 1463 | 1463 |
| $\mathrm{C} 6-\mathrm{N} 1$ | 1421 | 1421 |
| pyrimidine | 1385 | 1407 |
| C6-NH2 deformation | 1280 | - |
|  | 1198 |  |
| ribose C-O stretching vibration | 1102 |  |
|  | 1036 |  |
| P-O-H vibration | 1062,985 |  |

Table S2. During the synthesis process for the Sn -AMP samples, the pH of the solutions after hydrothermal treatment.

|  | Sn-AMP | Sn-125 | Sn-AMP $_{0.25}$ | Sn-AMP $_{0.5}$ |
| :---: | :---: | :---: | :---: | :---: |
| pH | 1.29 | 1.34 | Sn-AMP $_{0.75}$ |  |

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

| Entry | Catalyst | $\mathrm{X}(\%)$ | $\mathrm{Y}_{\text {HMF }}(\%)$ | $\mathrm{Y}_{\text {fructose }}(\%)$ | $\mathrm{Y}_{\mathrm{FA}}(\%)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | $\mathrm{Sn}-\mathrm{AMP}_{0.125}$ | 95.7 | 54.0 | 4.2 | 1.8 |
| 2 | $\mathrm{Sn}_{\mathrm{H}} \mathrm{AMP}_{0.25}$ | 96.8 | 62.1 | 5.0 | 2.1 |
| 3 | $\mathrm{Sn}^{-\mathrm{AMP}_{0.5}}$ | 96.4 | 63.5 | 4.1 | 2.0 |
| 4 | Sn-AMP | 0.75 | 97.1 | 56.4 | 3.1 |

Reaction condition: glucose ( 200 mg ), Sn -AMP ( 50 mg ), 5 mL of solvent, water/THF (v:v 1:4), $160^{\circ} \mathrm{C}$, 5 h .
Table S4. Comparison of Sn -AMP with other catalysts. (Yield: HMF yield, Sel.: HMF selectivity)

| saccharide | Solvent | Catalyst | T/ ${ }^{\circ} \mathrm{C}$ | $\mathrm{t} / \mathrm{h}$ | Yield | Sel. | Ref. |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ucrose |  |  | 170 | 4 | 61.6\% | $\geq 64.8 \%$ |  |
| glucose | water/DMSO/HCL | $\mathrm{Sn}-\mathrm{CP}$ | 170 | 4 | 63.9\% | 65.4\% | S3 |
| sucrose glucose | water/THF/ NaCl | Sn-Mont | 160 | 3 | $\begin{aligned} & \hline 43.6 \% \\ & 41.7 \% \end{aligned}$ |  | S4 |
| sucrose <br> glucose | water/Dioxane | Sn- $\beta$ /Amberlyst-131 | 90 | $\begin{aligned} & 10 \\ & 16 \end{aligned}$ | $\begin{aligned} & 60.0 \% \\ & 56.0 \% \end{aligned}$ |  | S5 |
| sucrose <br> glucose | water/THF/ NaCl | Phosphated $\mathrm{TiO}_{2}$ | 175 | $\begin{aligned} & 2 \\ & 4 \end{aligned}$ | $\begin{aligned} & 43.0 \% \\ & 53.5 \% \end{aligned}$ | $\begin{aligned} & 45.3 \% \\ & 54.3 \% \end{aligned}$ | S6 |
| sucrose <br> glucose | water /GVL/ NaCl | APG- $\mathrm{SO}_{3} \mathrm{H}$ | 180 | 4 | $\begin{aligned} & \hline 56.2 \% \\ & 52.9 \% \end{aligned}$ |  | S7 |
| sucrose <br> glucose | water/THF | [MimAM]nH3-nPW ${ }_{12} \mathrm{O}_{40}$ | 160 | 7.5 | $\begin{aligned} & \hline 23.5 \% \\ & 39.2 \% \end{aligned}$ | $\begin{aligned} & \hline 24.9 \% \\ & 39.5 \% \end{aligned}$ | S8 |
| sucrose <br> glucose | water/THF <br> water/THF | $\mathrm{Sn}-\mathrm{AMP}_{0.5}$ | $\begin{aligned} & 160 \\ & 160 \end{aligned}$ | 4.5 5 | $\begin{aligned} & \hline 62.9 \% \\ & 67.5 \% \end{aligned}$ | $\begin{aligned} & \hline 63.0 \% \\ & 69.6 \% \end{aligned}$ | This work |

## References

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