nanomaterials

SUPPORTING INFORMATION

Metal-Free Phosphated Mesoporous SiO_2 as Catalyst for the Low-Temperature Conversion of SO_2 to H_2S in Hydrogen

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Table S1. XPS elemental concentrations for uf-P@m-SiO_2-cal (A: fresh), and uf-P@m-SiO_2 (B: fresh, and C: used).

Element	Atomic %		
	uf-P@m-SiO_2-cal	**uf-P@m-SiO_2 (Fresh)**	**uf-P@m-SiO_2 (Used)**
C	20.3	20.6	16.7
N	0.9	0.9	0.7
O	53.4	53.1	56.0
Si	25.2	25.3	26.5
P	0.1	0.1	0.1

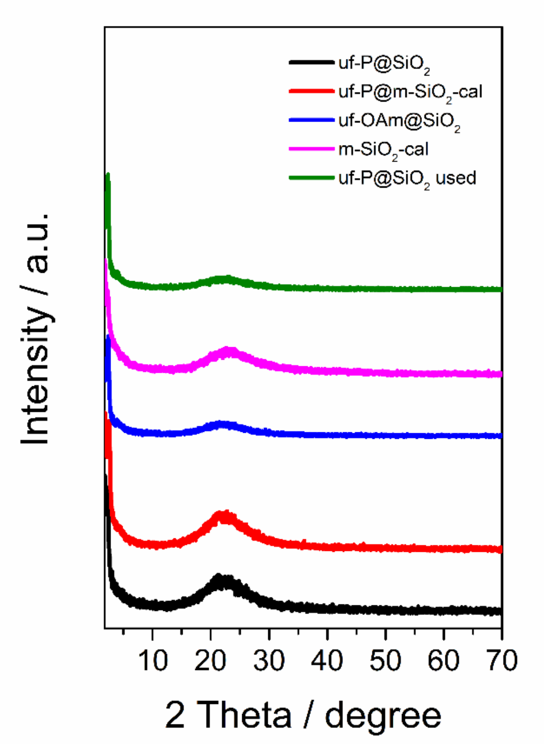


Figure S1. XRD patterns uf-P@m-SiO_2 (fresh and used), uf-P@m-SiO_2-cal, uf-OAm@m-SiO_2, and m-SiO_2-cal.

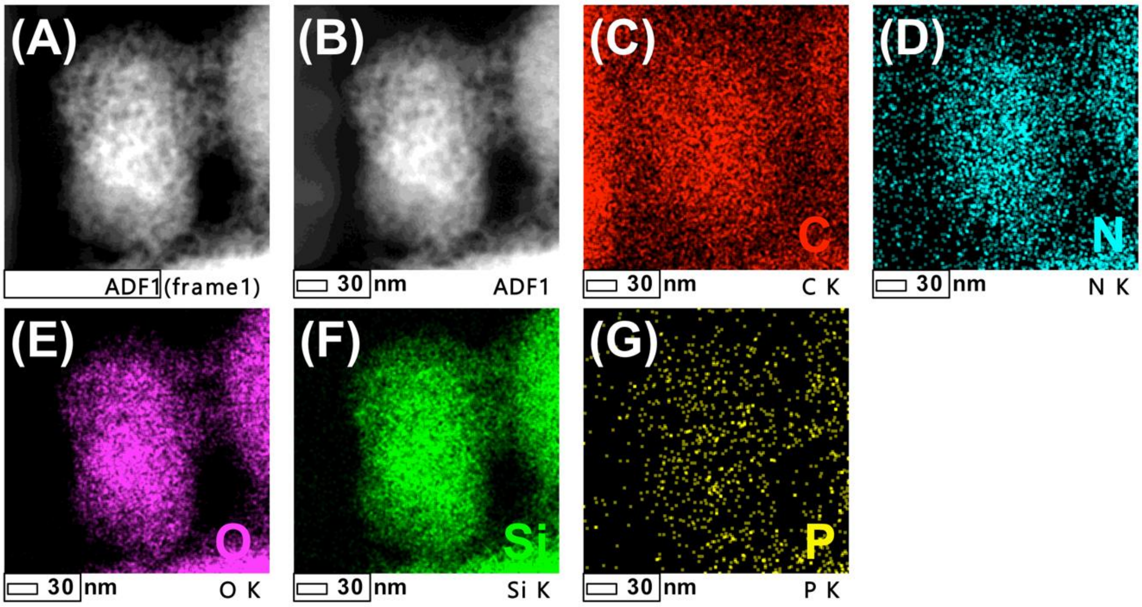


Figure S2. TEM elemental mapping of uf-P@m-SiO_2 (Position 2). (**A**,**B**) the TEM image of uf-P@m-SiO2, (**C**) the C element mapping, (**D**) the N element mapping, (**E**) the O element mapping, (**F**) the Si element mapping (**G**) the P element mapping.

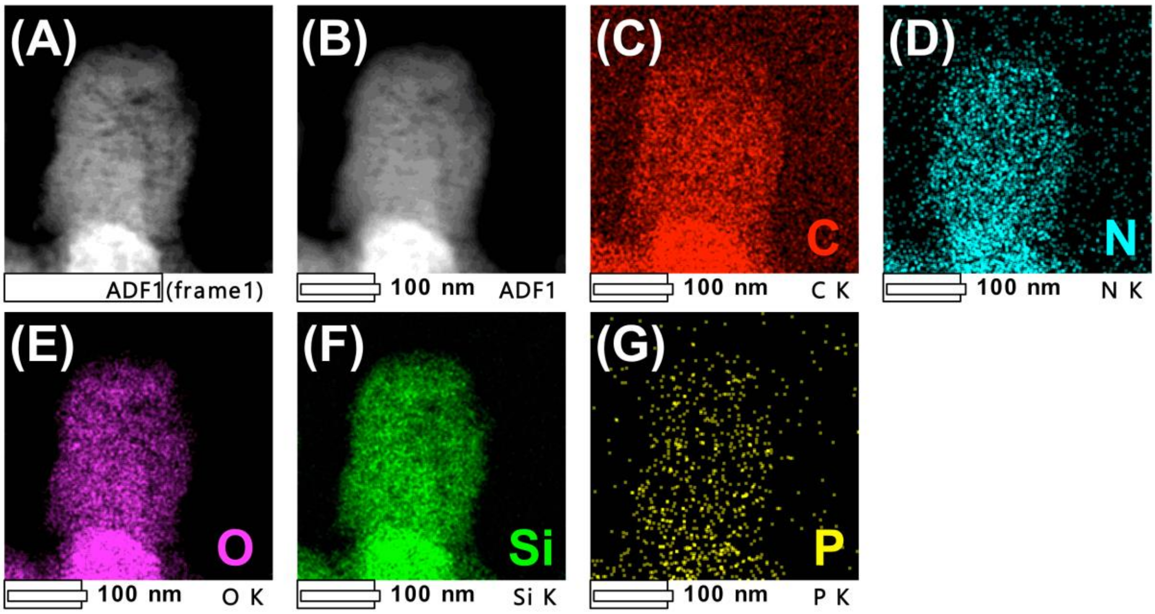
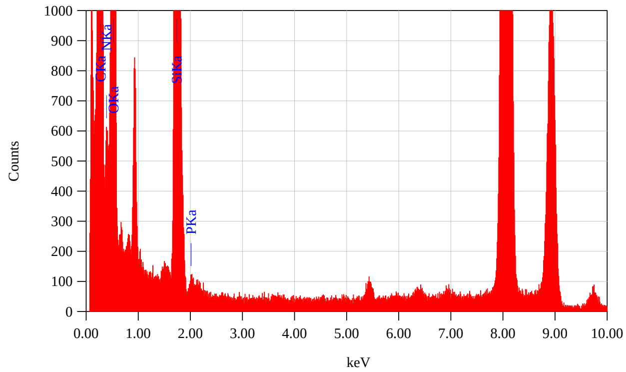
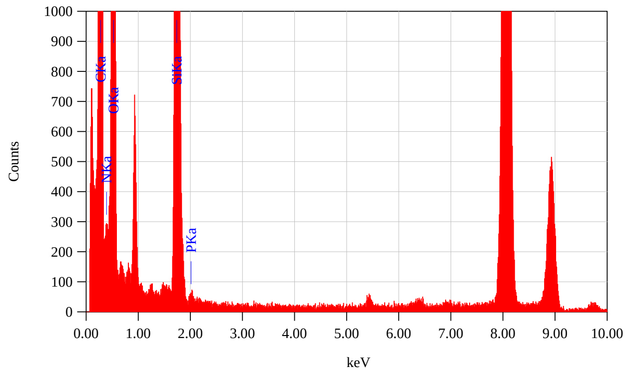


Figure S3. TEM elemental mapping of uf-P@m-SiO_2 (Position 3). (**A**,**B**) the TEM image of uf-P@m-SiO2, (**C**) the C element mapping, (**D**) the N element mapping, (**E**) the O element mapping, (**F**) the Si element mapping (**G**) the P element mapping.

Position 1. (corresponding to Figure 5)



Position 2. (corresponding to Figure S2)



Position 3. (corresponding to Figure S3)

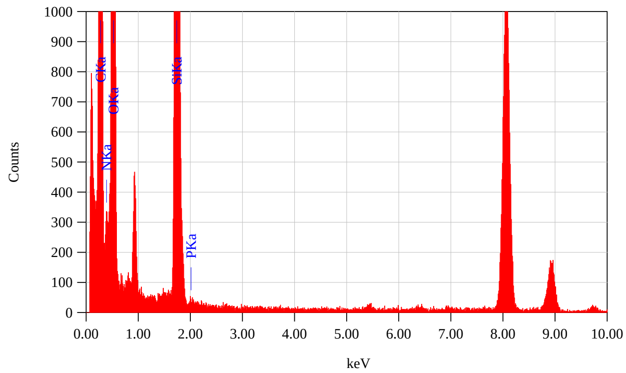


Figure S4. TEM-EDX total area spectrum recorded from the mapped area in Figure 5, Figure S2, and Figure S3 for the sample uf-P@m-SiO_2.

Table S2. TEM-EDX elemental concentrations for uf-P@m-SiO_2.

Element	Atomic %		
	Position 1	**Position 2**	**Position 3**
C	74.97	70.53	67.31
N	0.60	0.51	0.68
O	16.83	19.87	22.41
Si	7.57	9.05	9.58
P	0.03	0.03	0.03

Table S3. Weisz-Prater Criterion and Mears Criterion calculation for the catalyst performance test.

Weisz-Prater Criterion	
R (Catalyst particle radius, cm)	2.0E-02
ρ_c (catalyst density, g cm^{-3})	1.6E-02
C_{As} (Gas concentration at the catalyst surface, mol cm^{-3})	4.5E-05
D_c (Effective diffusivity cm^2 s^{-1})	1.0E-05
$r_{A\ obs}$ (mol g^{-1} s^{-1})	1.0E-07
C_{wp}	1.4E-02
Mears Criterion	
n (reaction order)	1
R (Catalyst particle radius, cm)	2.0E-02
ρb (bulk catalyst density, g cm^{-3})	8.7E-01
k c (mass transfer coefficient cm s^{-1})	5.3
C_{Ab} (bulk gas concentration mol cm^{-3})	4.5E-05
rA $_{obs}$ (mol g^{-1} s^{-1})	1.0E-07
C_M	7.4E-06

The Weisz-Prater Criterion is far below 1, and Mears Criterion is far below 0.15, so the diffusion of reactants to the catalyst were negligible. [16, 28-29]

Table S4. Comparison of the catalytic performance of different catalysts from literature of the SO_2 conversion to H_2S, selectivity and yield of H_2S.

Catalyst	T (°C)	SO_2 Conv. (%)	H_2S Select. (%)	H_2S Yield (%)	Reference
NiO/r-Al_2O_3	320	98	31	30.4	[30]
SnO_2-ZrO_2	550	98	45	44.1	[31]
Fe/γ-Al_2O_3	240	100	100	100	[9]
Fe-Si-Cr	190	100	100	100	[32]
l-Ni_5P_4@SiO_2	325	96	99	95	[17]
u-Ni_5P_4@SiO_2-l	240	97	34	33	[17]
uf-P@m-SiO_2	140	18	6	1	This work
uf-P@m-SiO_2	160	50	8	4	This work
uf-P@m-SiO_2	180	76	33	25	This work
uf-P@m-SiO_2	200	91	39	35	This work
uf-P@m-SiO_2	220	94	52	49	This work
uf-P@m-SiO_2	240	96	52	50	This work

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