Supporting information for

Bamboo derived activated carbon as highly efficient catalysts for the oxidation and adsorption of hydrogen sulfide at room temperature

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Fig. S13. The optimized geometries of the intermediates and transition states.

Text S1. The equations of Yoon and Nelson model, Diffusion model and Adsorption kinetics models.

The Yoon and Nelson model (Y-N) can be expressed as following:

$$\frac{C_0}{C_i} = \frac{1}{1 + exp\left[k'(t_0 - t)\right]}$$

Where the outlet and inlet concentrations of the stream are marked as C_o and C_i, respectively. While t_0 is the time for 50% adsorbate breakthrough (min), and k' is a rate constant (min^{-1}).

The Pseudo first order kinetic model (PFO) can be expressed as following:

$$q_t = q_e(1 - e^{-k_1 t})$$

Where k_1 (min^{-1}) is the kinetic constant of PFO adsorption, q_e (mg/g) and q_t (mg/g) are the amount of D4 adsorption at equilibrium and at time t (min), respectively.

The Pseudo second order kinetic model (PSO) can be expressed as following:

$$q_t = \frac{q_e t}{t + \frac{1}{q_e k_2}}$$

Where k_2 (min^{-1}) is the kinetic constant of PSO adsorption, q_e (mg/g) and q_t (mg/g) have the same meaning as before.

The Intra-particle diffusion model (IPD) can be expressed as following:

$$q_e = k_{id} t^{0.5} + \theta$$

Where k_{id} ($mg/g \cdot min^{-0.5}$) is the intra-particle-diffusion rate constant, θ (mg/g) is a constant related to the thickness of the boundary layer.

The Linear driving force model (LDF) can be expressed as following:

$$\frac{M_t}{M_e} = 1 - e^{-kt}$$

Where *Mt* (mg/g) is the adsorption capacity at time t; *Me* (mg/g) is the equilibrium adsorption capacity of a given pressure increment, and *k* (min^{-1}) is the rate constant.

TableS1 The parameters of different models of Na/BAC catalysts

Model	Parameter	Na/BAC-2	Na/BAC-4	Na/BAC-6	Na/BAC-8
Pseudo first order **(PFO)**	Q_e (g $H_2S \cdot$ g cat^{-1})	0.154	0.348	0.565	0.791
	k_1 (min^{-1})	0.002	0.002	0.001	0.0006
	R^2	0.995	0.978	0.983	0.994
Pseudo Second Order **(PSO)**	Q_e (g $H_2S \cdot$ g cat^{-1})	0.154	0.354	0.572	0.793
	k_2 ($g \cdot g^{-1} \cdot min^{-1}$)	0.0019	0.002	0.0007	0.0001
	R^2	0.984	0.963	0.970	0.974
Intra-particle diffusion **(IPD)**	k_{iP} ($g \cdot g^{-1} \cdot min^{-0.5}$)	0.0076	0.009	0.013	0.005
	C ($g \cdot g^{-1}$)	-0.017	-0.022	-0.042	-0.008
	R^2	0.957	0.956	0.954	0.963
Linear driving force **(LDF)**	k	0.009	0.004	0.003	0.002
	R_2	0.928	0.933	0.936	0.926
Yoon and Nelson model **(Y-N)**	k	0.046	0.016	0.015	0.011
	R_2	0.908	0.980	0.953	0.993

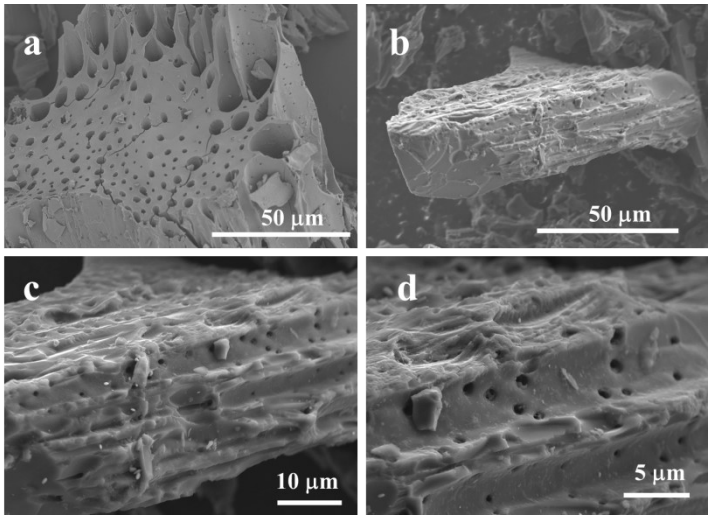

Fig.S1 SEM image of Na/BAC-8

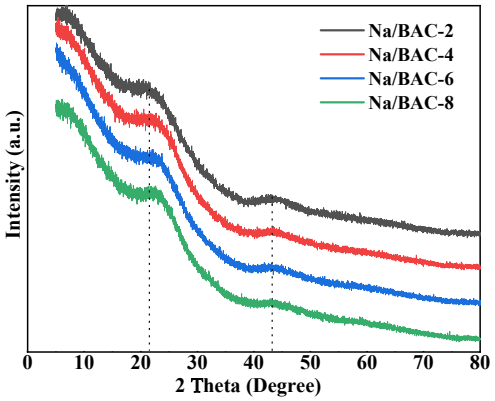

Fig.S2 XRD patterns of Na/BAC catalysts

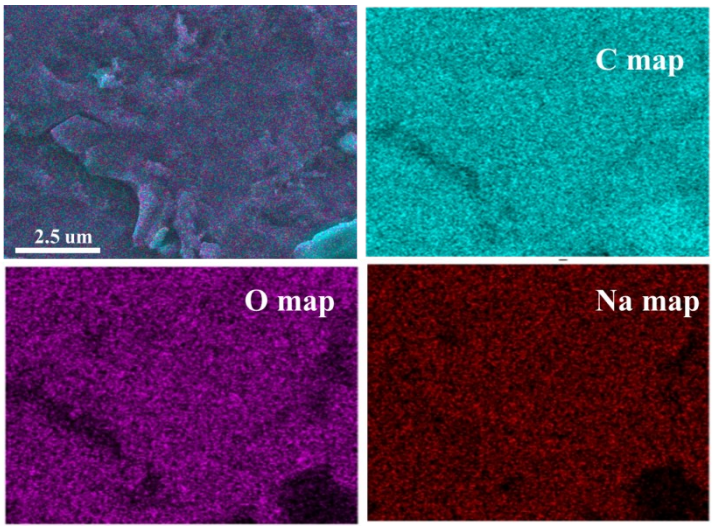

Fig.S3 EDS mapping of Na/BAC-8

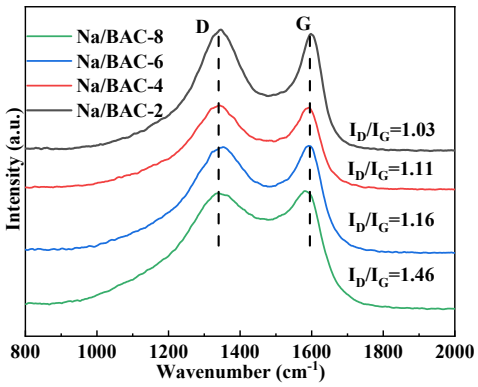

Fig.S4 Raman spectra of Na/BAC catalysts

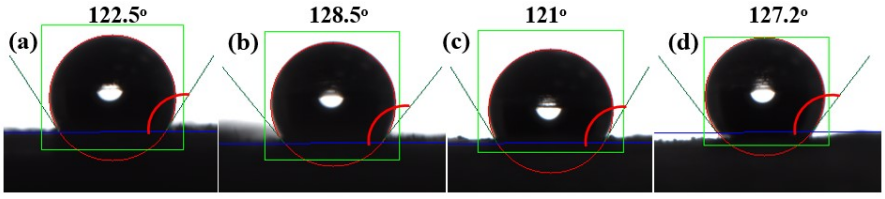

Fig.S5 contact angle image of (a) Na/BAC-2 (b) Na/BAC-4(c) Na/BAC-6 (d) Na/BAC-8

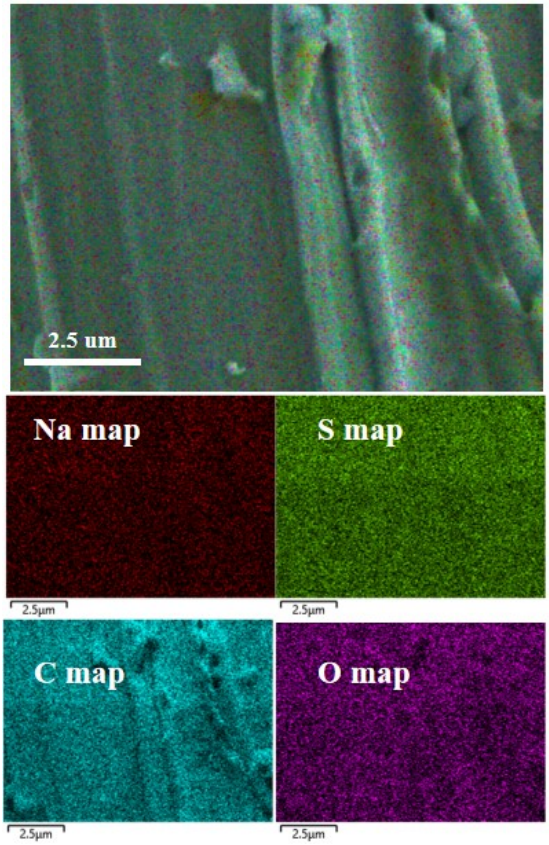

Fig.S6 EDS mapping of spent Na/BAC-8 catalyst

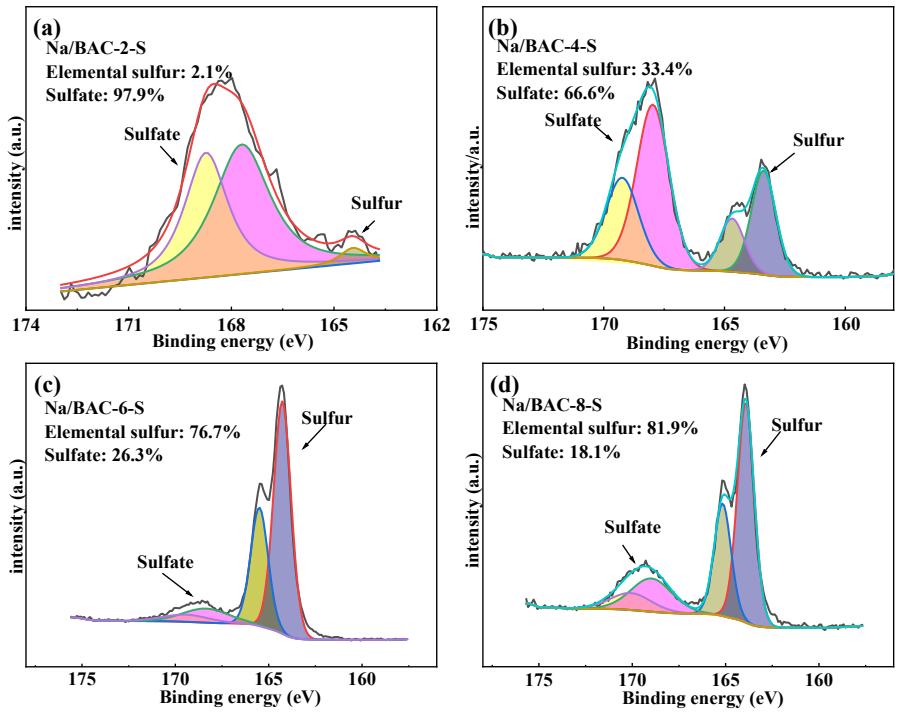

Fig. S7 S 2p XPS spectra of spent Na/BAC catalyst

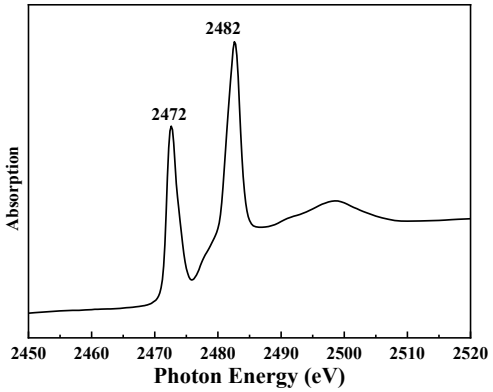

Fig.S8 Sulfur K-edge XANES spectra of spent Na/BAC-8 catalyst

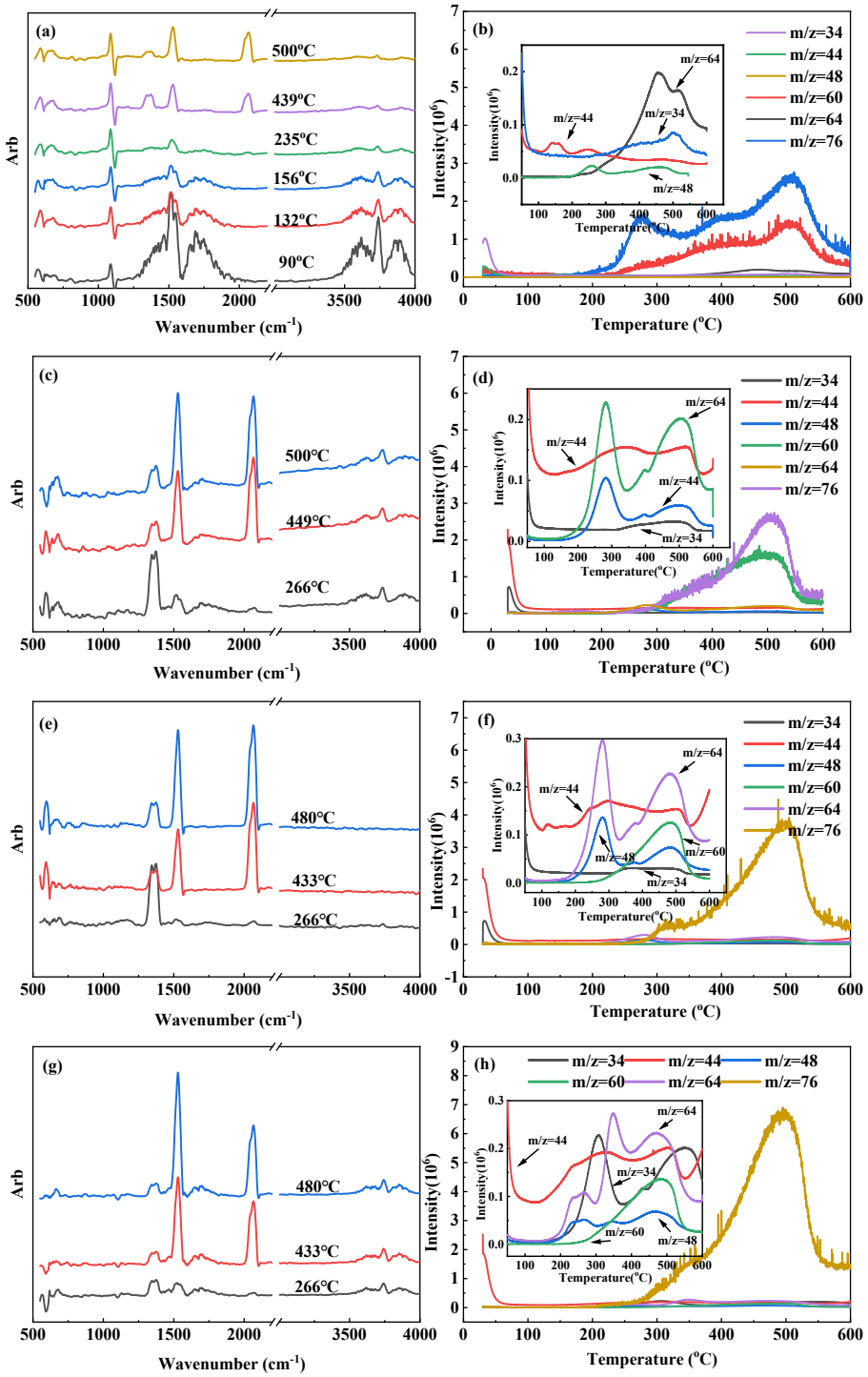

Fig.S9 IR spectra at different temperature (a) Na/BAC-2, (c) Na/BAC-4, (e) Na/BAC-6, (g) Na/BAC-8 and MS profiles (b) Na/BAC-2, (d) Na/BAC-4, (f) Na/BAC-6, (h) Na/BAC-8 of spent Na/BAC catalysts

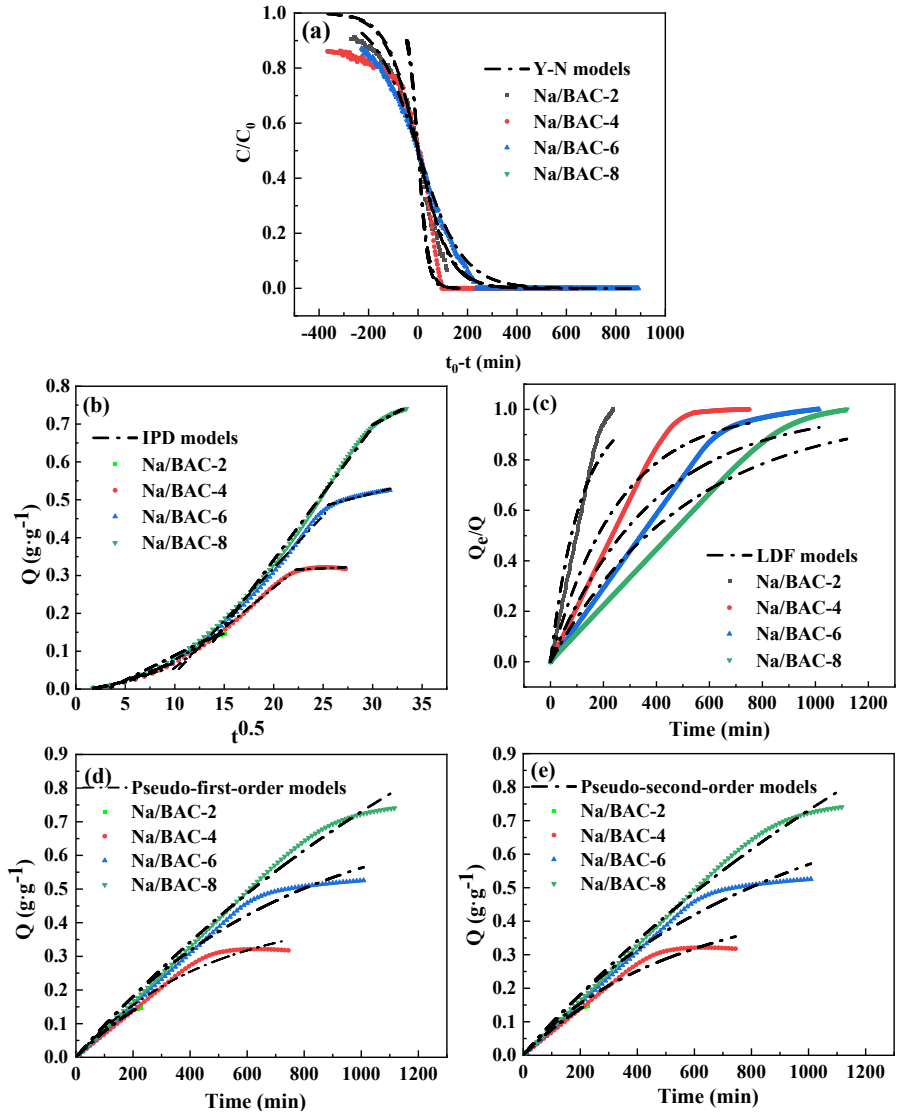

Fig.S10 Y-N models (a), IPD models (b), LDF models (c), PFO models (d) and PSO models (e) fitting of Na/BAC catalysts.

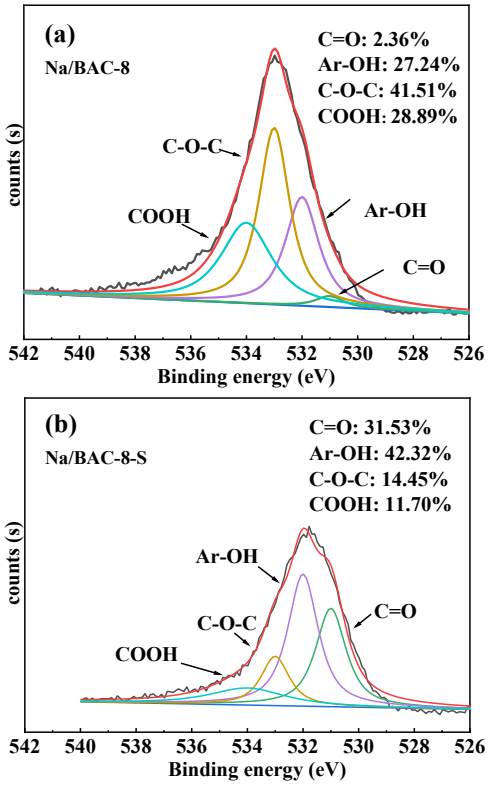

Fig.S11 The O1s XPS spectra of Na/BAC-8 (a) and Na/BAC-8-S (b)

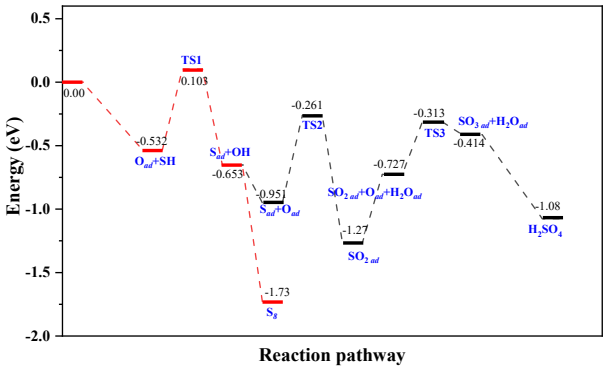

Fig. S12 Energy profile of H_2S catalytic oxidation-adsorption at room temperature

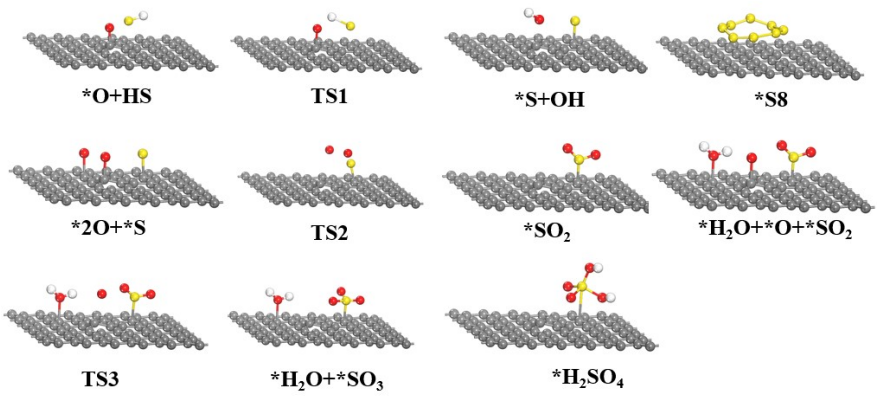

Fig.S13 The optimized geometries of the intermediates and transition states