Design of Sn-doped MoS_2 piezocatalyst for high-efficiency antibiotic degradation: mechanism and performance

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Text S1 Materials and chemicals

Ammonium molybdate ($H_{24}Mo_7N_6O_{24}\cdot 4H_2O$, 99%), thioacetamide ($C_2H_5NS$, 99%), Tin tetrachloride ($SnCl_4$), disodium ethylenediamine tetraacetate (EDTA-2Na, $C_{10}H_{14}N_2Na_2O_8$), polyether P123 ($H(OCH_2CH_2)_x(OCH_2CH_3)_y(OCH_2CH_2)_zOH$), tert-butanol (TBA, $C_{19}H_{15}F_3N_4O_5$, ≥98%), benzoquinone (BQ, $C_4H_{10}O$, 99.5%), silver nitrate ($AgNO_3$), sodium chloride (NaCl, 99.5%), sodium nitrates (Na_2NO_3, ≥99.5%), calcium carbonate ($CaCO_3$, ≥99.5%), and sodium sulfate (Na_2SO_4) were purchased from McLean Chemical Reagents Limited and were analytically pure, requiring no further purification, and the deionized water was prepared by the laboratory itself.

Text S2 Characterization and analysis methods

The prepared samples were characterized for morphology and structure using scanning electron microscopy (SEM, regulus 8100) and transmission electron microscopy (TEM, JEM-2100PLUS). The elemental composition and distribution of the samples were analyzed by energy dispersion X-ray spectroscopy (EDS, regulus 8100). X-ray diffraction (XRD, D/MAX/2500PC), X-ray photoelectron spectroscopy (XPS, AXIS SUPRA), and Raman spectroscopy (Raman, invia Qontor) were employed to characterize the chemical structure of the material surface. Electron paramagnetic resonance (EPR, EPR200-Plus) was utilized to compare the relative number of free radicals. The electrochemical properties of the samples were measured using an electrochemical workstation (DH7002A). Atomic force microscopy (PFM, Bruker Dimension ICON) was used to study both the morphology and piezoelectric properties of the sample. For PFM measurement purposes, the powder sample was dispersed in an

ethanol solvent before being coated on a Pt/Si substrate.

Text S3 Piezo-electrochemical performance measurements

Under ultrasonic vibration and dark conditions, the piezoelectric electrochemical performance of the sample was monitored using a traditional three-electrode system using an electrochemical workstation (DH7002A). Disperse 3 mg of sample into 770 μL of pure water, 200 μL of ethanol, and 30 μL of naphthol. Completely drip the mixture onto carbon cloth (CP) (1×1 cm^2) on a surface and dry in the air for 24 hours. Use platinum sheets as counter electrodes. Ag/AgCl is used as the reference electrode, carbon cloth (CP) is used as the working electrode, and a newly prepared KOH solution (mol L^{-1}) is used as the electrolyte.

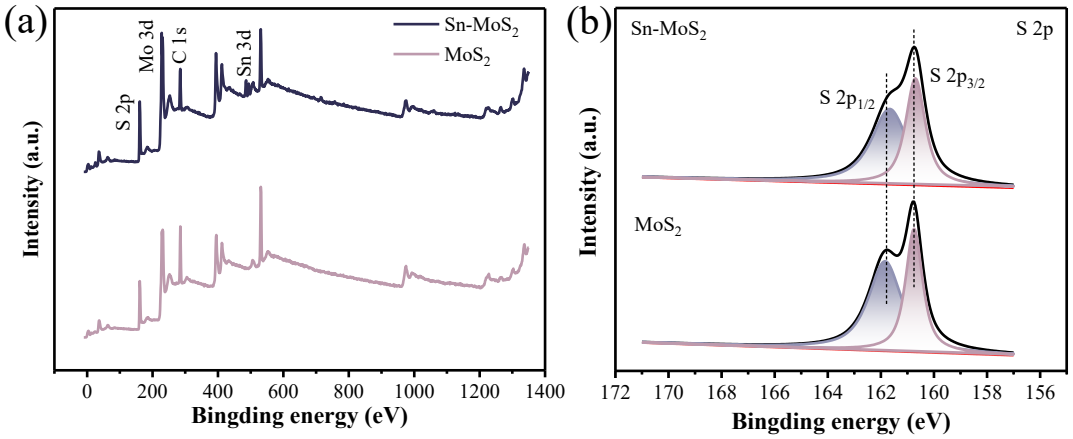


Fig. S1. (a) Scanning spectra and high-resolution scans of the (b) S 2p of MoS_2 and Sn-MoS_2.

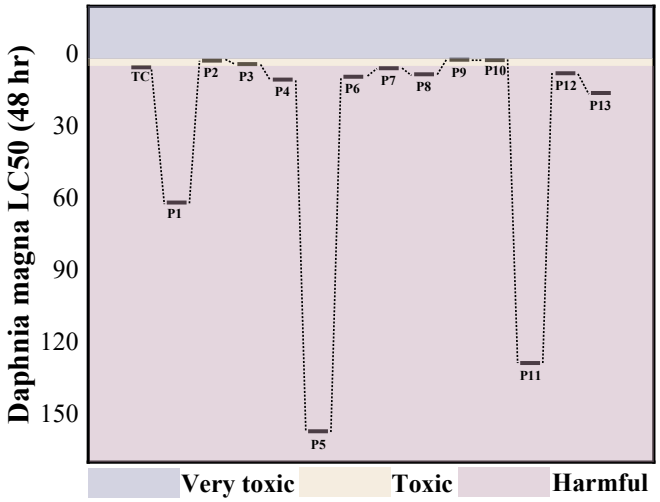


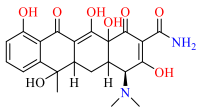
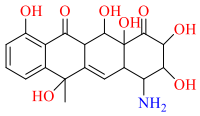
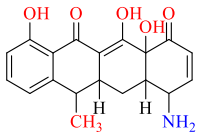
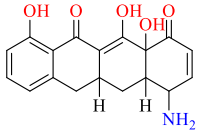
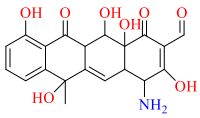
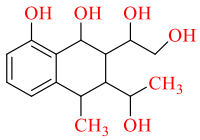
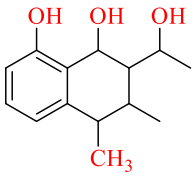
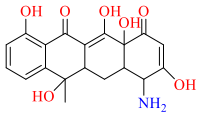
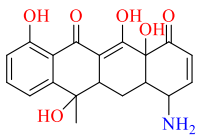
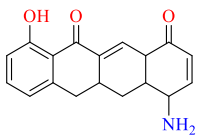
Fig. S2. Acute toxicity (48 h LC50)

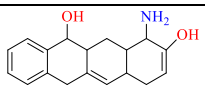
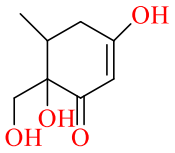
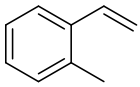
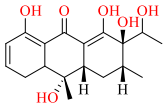
Table S1 Fukui values of atoms in TC molecule.

Atom	q(N)	q(N+1)	q(N-1)	$f^{(-)}$	$f^{(+)}$	$f^{(0)}$	CDD
C (1)	0.051	0.101	0.002	0.003	0.104	0.054	0.101
C (2)	0.022	0.038	0.006	0.005	0.006	0.006	0.001
C (3)	0.055	0.101	0.009	0.011	0.115	0.063	0.104
C (4)	0.006	0.009	0.003	-0.003	-0.012	-0.007	-0.009
C (5)	0.002	0.003	0.001	-0.006	-0.011	-0.008	-0.005
C (6)	0.005	0.006	0.005	-0.005	-0.008	-0.007	-0.003
C (7)	0.004	0.003	0.005	-0.009	-0.008	-0.009	0.001
C (8)	0.002	0.001	0.003	-0.011	-0.005	-0.008	0.006
C (9)	0.015	0.001	0.028	0.015	0.002	0.008	-0.013
C (10)	0.039	0.012	0.066	0.049	0.006	0.028	-0.043
C (11)	0.031	0.021	0.04	0.016	0.011	0.013	-0.005
C (12)	0.034	0.016	0.053	0.038	0.01	0.024	-0.028
C (13)	0.024	0.011	0.036	0.018	0.007	0.013	-0.011
C (14)	0.016	0	0.033	0.03	-0.002	0.014	-0.032
C (15)	0.019	0.015	0.022	0.017	0.014	0.016	-0.003
C (16)	0.025	0.017	0.032	0.025	0.021	0.023	-0.004
C (17)	0.015	-0.007	0.036	0.035	-0.007	0.014	-0.042
C (18)	0.006	0.007	0.004	-0.001	-0.012	-0.006	-0.011
C (19)	0.004	0.003	0.006	0.004	0.004	0.004	0
O (20)	0.035	0.04	0.029	0.031	0.046	0.038	0.015
N (21)	0.017	0.021	0.013	0.008	0.015	0.011	0.007
O (22)	0.051	0.025	0.078	0.081	0.024	0.053	-0.057
O (23)	0.067	0.119	0.015	0.015	0.12	0.068	0.105
C (24)	0.005	0.003	0.007	-0.006	-0.004	-0.005	0.002
O (25)	0.023	0.038	0.009	0.005	0.035	0.02	0.03
O (26)	0.031	0.012	0.05	0.047	0.016	0.032	-0.031
O (27)	0.057	0.021	0.092	0.097	0.023	0.06	-0.074
O (28)	0.016	0.009	0.023	0.024	0.01	0.017	-0.014
O (29)	0.049	0.078	0.019	0.019	0.074	0.046	0.055
N (30)	0.003	0.003	0.003	-0.001	-0.012	-0.007	-0.011
C (31)	0.006	0.009	0.003	-0.007	-0.015	-0.011	-0.008
C (32)	0.004	0.006	0.002	-0.004	-0.013	-0.009	-0.009
H (33)	0.005	0.007	0.003	0.008	0.019	0.013	0.011
H (34)	0.01	0.008	0.011	0.024	0.017	0.021	-0.007
H (35)	0.015	0.025	0.005	0.012	0.048	0.03	0.036
H (36)	0.007	0.007	0.007	0.015	0.015	0.015	0
H (37)	0.01	0.011	0.01	0.021	0.02	0.021	-0.001
H (38)	0.019	0.009	0.03	0.054	0.018	0.036	-0.036
H (39)	0.021	0.014	0.029	0.056	0.026	0.041	-0.03
H (40)	0.021	0.013	0.03	0.057	0.024	0.04	-0.033

H (41)	0.008	0.009	0.006	0.008	0.01	0.009	0.002
H (42)	0.017	0.023	0.011	0.018	0.037	0.028	0.019
H (43)	0.002	0.001	0.003	0.005	0.001	0.003	-0.004
H (44)	0.009	0.002	0.016	0.031	0.004	0.018	-0.027
H (45)	0.011	0.011	0.01	0.019	0.022	0.02	0.003
H (46)	0.014	0.013	0.014	0.019	0.017	0.018	-0.002
H (47)	0.012	0.009	0.015	0.017	0.012	0.015	-0.005
H (48)	0.015	0.006	0.024	0.024	0.008	0.016	-0.016
H (49)	0.008	0.005	0.011	0.015	0.007	0.011	-0.008
H (50)	0.014	0.021	0.007	0.011	0.024	0.018	0.013
H (51)	0.012	0.016	0.009	0.018	0.03	0.024	0.012
H (52)	0.006	0.011	0	-0.002	0.022	0.01	0.024
H (53)	0.006	0.008	0.005	0.01	0.014	0.012	0.004
H (54)	0.004	0.011	-0.002	-0.007	0.021	0.007	0.028
H (55)	0.013	0.016	0.009	0.019	0.032	0.026	0.013
H (56)	0.002	0.002	0.002	0.004	-0.001	0.001	-0.005

Table S2 Information on intermediates.

Compound	m/z	Formula	Supposed structure	Daphnia magna LC50 (48 hr)	Bioaccumulation factor	Developmental toxicity	Mutagenicity
TC	445	$C_{22}H_{24}N_2O_8$		5.44	0.71	0.86	0.60
P1	392	$C_{22}H_{24}N_2O_9$		61.78	10.59	0.69	0.73
P2	341	$C_{19}H_{19}NO_5$		2.62	1.59	0.84	0.70
P3	328	$C_{18}H_{17}NO_5$		4.07	1.16	0.89	0.58
P4	416	$C_{20}H_{19}NO_8$		10.57	N/A	0.78	0.69
P5	282	$C_{15}H_{22}O_5$		157.13	3.70	0.64	0.42
P6	237	$C_{14}H_{20}O_3$		9.37	26.80	0.73	0.43
P7	373	$C_{19}H_{19}NO_7$		5.82	1.20	0.79	0.78
P8	357	$C_{19}H_{19}NO_6$		8.35	0.80	0.83	0.78
P9	296	$C_{18}H_{17}NO_3$		2.27	3.84	1.03	0.61

P10	283	$C_{18}H_{21}NO_2$		2.41	23.66	0.93	0.62
P11	172	$C_8H_{12}O_4$		128.70	0.39	0.54	0.61
P12	119	C_9H_{10}		7.90	112.01	0.49	N/A
P13	212	$C_{13}H_{24}O_2$		16.16	27.62	0.75	N/A