Supporting information

One-step synthesis of pure-phase amino-functionalized zirconium-based capsule ZrC-1-NH_2 for photocatalytic degradation of tetracycline

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Table. S1. Crystal data and structure refinement for ZrC-1-NH_2

Identification code	ZrC-1-NH_2
Empirical formula	$C_{54}H_{48}Cl_2N_3O_{21}Zr_6$
Formula weight	1693.17
Temperature/K	150.0
Crystal system	Orthorhombic
Space group	Cmcm
a/Å	19.8615(12)
b/Å	17.7218(10)
c/Å	17.2448(12)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	6069.9(7)
Z	4
$\rho_{calc}g/cm^3$	1.853
μ/mm^{-1}	6.389
F(000)	3340.0
Crystal size/mm^3	0.21 × 0.2 × 0.19
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	5.814 to 137.288
Index ranges	$0 \le h \le 22$, $-24 \le k \le 24$, $-21 \le l \le 0$
Reflections collected	6307
Independent reflections	3322 [R_{int} = 0.0438, R_{sigma} = 0.0486]
Data/restraints/parameters	3322/66/215
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0680, wR_2 = 0.1990
Final R indexes [all data]	R_1 = 0.0716, wR_2 = 0.2027
Largest diff. Peak/hole/ $eÅ^{-3}$	1.76/-1.36

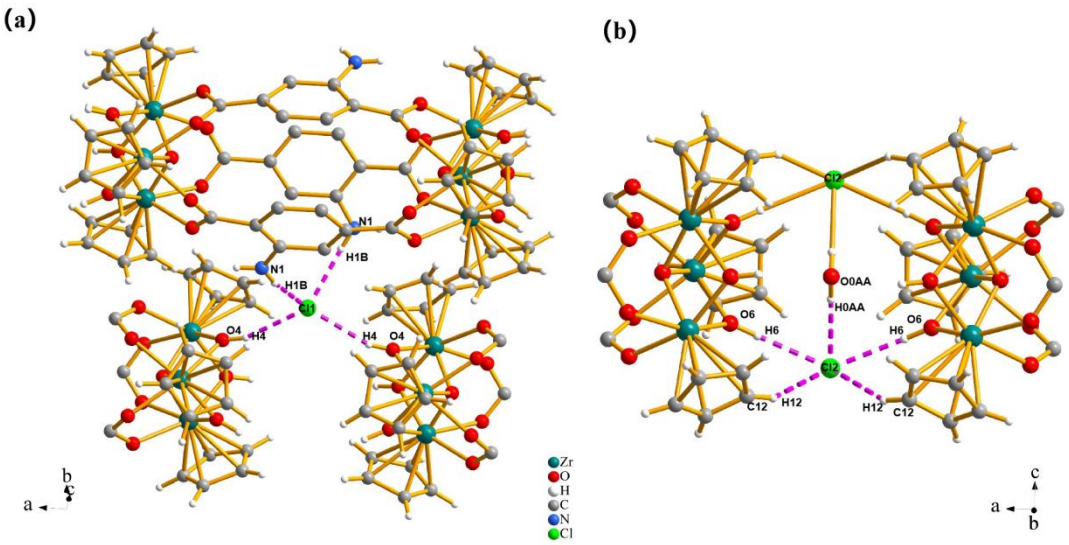

Fig. S1. Coordination environment diagrams of Cl1 (a) and Cl2 (b), aiming to emphasize the multiple hydrogen bonds within the structure, where the occupancy of Cl1 is 1 and that of Cl2 is 0.5. For clarity, the hydrogen atoms on the benzene ring of the ligand are omitted.

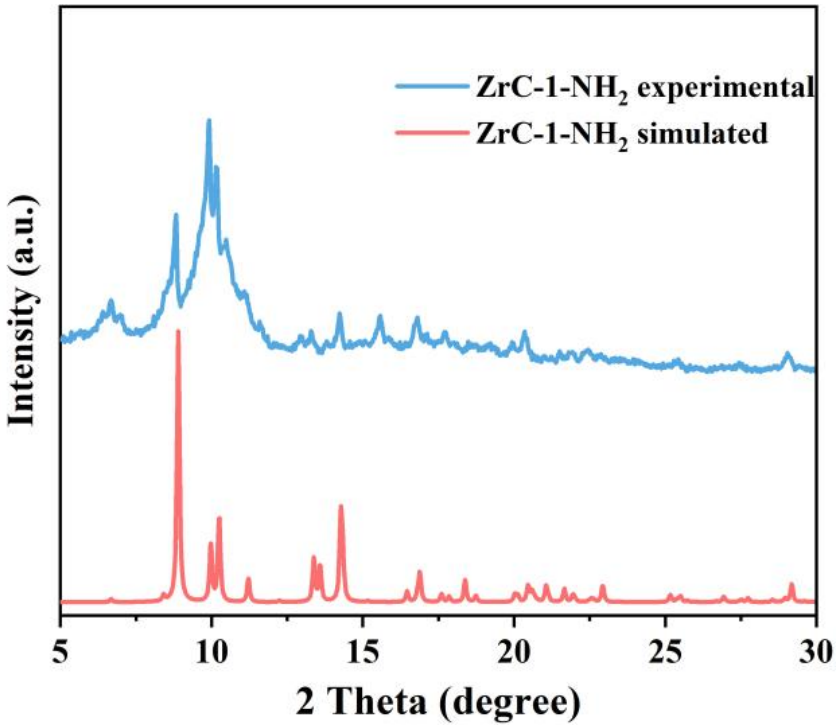

Fig. S2 PXRD patterns of ZrC-1-NH_2.

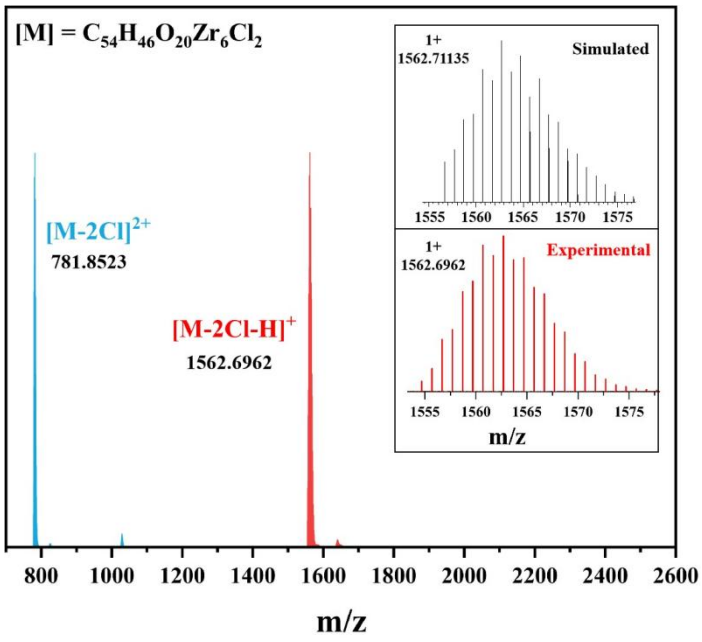

Fig.S3. ESI-TOF-MS of MW-ZrC-1

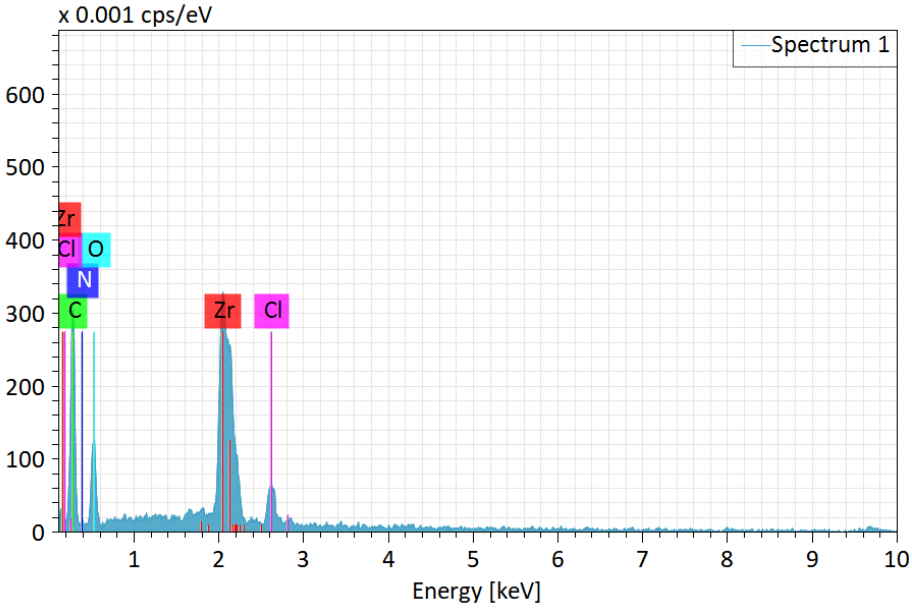

Fig. S4. EDS spectrum of MW-ZrC-1-NH_2

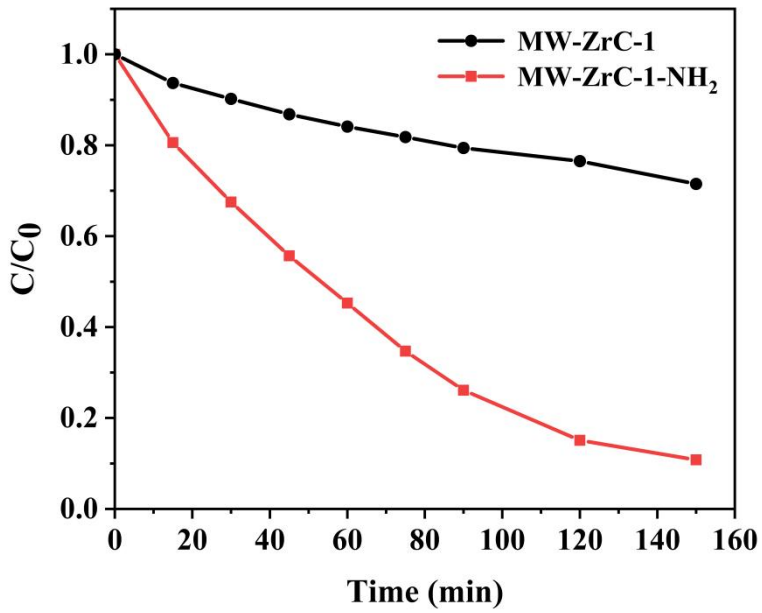

Fig. S5. Comparison of photocatalytic degradation of tetracycline by MW-ZrC-1-NH_2 and MW-ZrC-1.

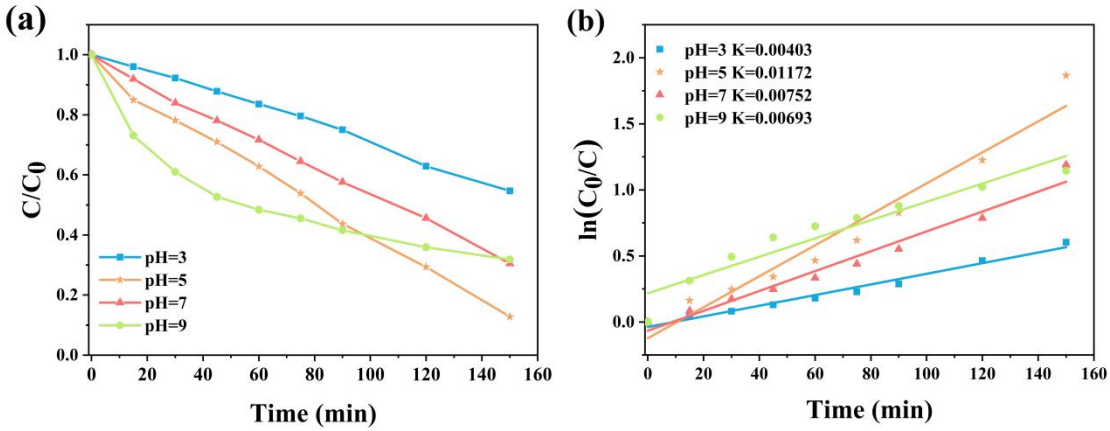

Fig. S6 (a) The removal efficiency of TC on different pH; (b) the kinetic curves of TC on different pH.

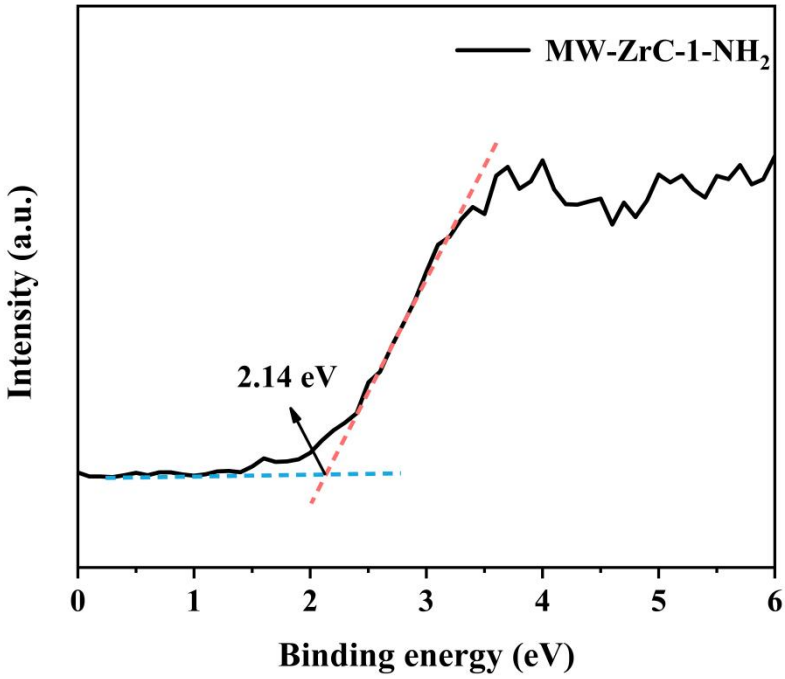

Fig. S7. VB-XPS spectra of MW-ZrC-1-NH_2.

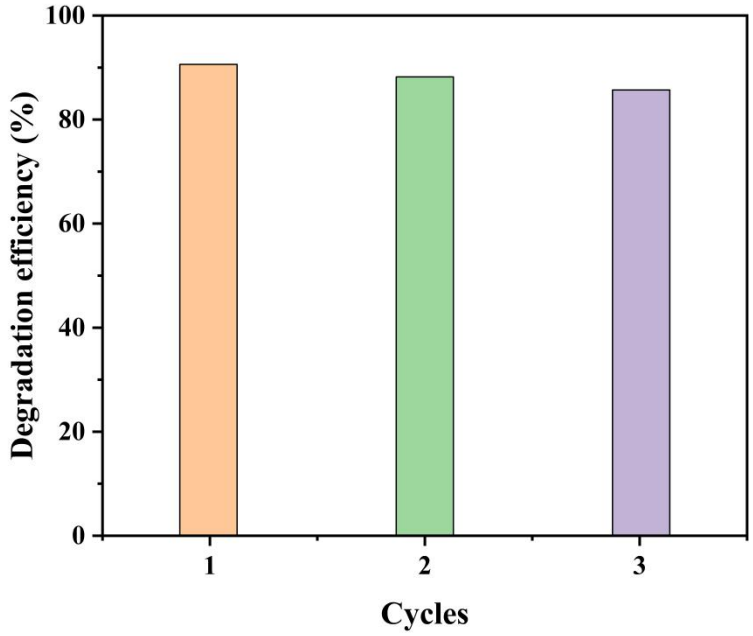

Fig. S8. The recycle experiments of MW-ZrC-1-NH_2 photocatalyst.

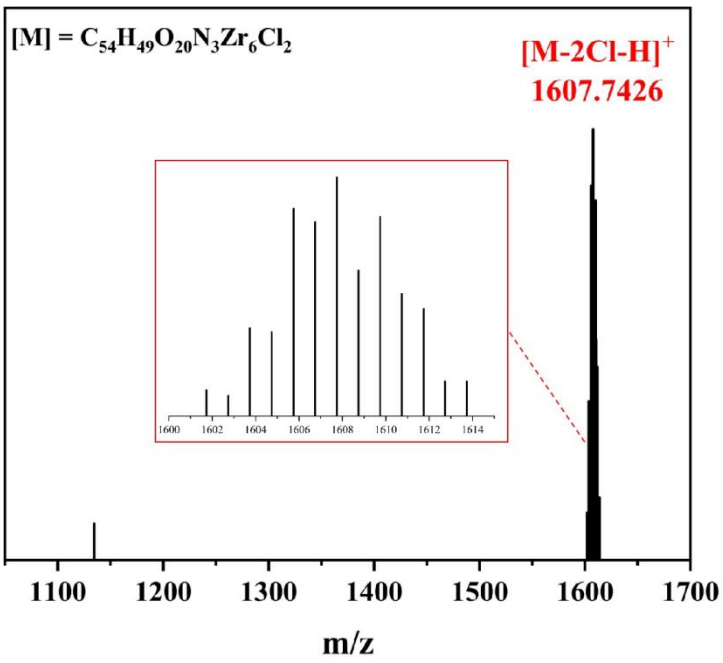

Fig. S9. The ESI-TOF-MS of MW-ZrC-1-NH_2 after photodegradation of TC.