Supporting Information

Construction of zirconium/hafnium–oxo clusters based on new protection–calix[8]arene

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General Experimental Section

All the reagents were obtained from commercial sources and used without further purification. Powder X-ray diffraction (PXRD) patterns were recorded ranging from 5 to 50º at room temperature on a Siemens D5005 diffractometer with Cu Kα (λ = 1.5418 Å). The C, H and N elemental analysis were conducted on a Perkin–Elmer 2400CHN elemental analyzer. Thermogravimetric analysis (TGA) of the samples were performed using a Perkin–Elmer TG–7 analyzer heated from room temperature to 800 ºC under nitrogen at the heating rate of 10 °C·min^{-1}. IR spectrum was performed in the range 4000–400 cm^{-1} using KBr pellets on an Alpha Centaurt FT/IR spectrophotometer.

Synthesis of Zr_4

A mixture of TBC[8] (40 mg), $ZrCl_4$ (40 mg) was dissolved in DMF (6 mL) and CH_3OH (6 mL). The mixture was transferred into a Parr Teflon–lined autoclave and kept at 130 °C for 72 h. After cooling down to room temperature, the colorless crystals were obtained and washed with CH_3OH. The crystals were achieved in a 43% yield based on TBC[8]. Elemental analysis (%): calculated for $[Zr_4Cl_2(H_2TBC[8])_2(HCOO)_2(CH_3OH)_4]\cdot 2CH_3OH\cdot 3DMF$, C 65.8, H 7.2, N 1.2; found, C 64.5, H 7.3, N 1.1.

Synthesis of Zr_8

A mixture of TBC[8] (100 mg), $ZrCl_4$ (50 mg) was dissolved in DMF (5 mL), CH_3OH(5 mL) and en (ethylenediamine, 1 mL). The mixture was transferred into a Parr Teflon–lined autoclave and kept at 130 °C for 72 h. After cooling down to room temperature, the colorless crystals were obtained and washed with CH_3OH. The crystals were achieved in a 35% yield based on TBC[8]. Elemental analysis (%): calculated for $[Zr_8(TBC[8])_2(\mu_4\text{-}O)_2(\mu_3\text{-}O)_4(\mu_3\text{-}OH)_2(\mu_2\text{-}OH)_2(H_2O)_2(DMF)_4]\cdot 8CH_3OH\cdot 7DMF$, C 57.1, H 7.0, N 3.3; found, C 56.2, H 6.6, N 3.2.

Synthesis of Hf_4

A mixture of TBC[8] (40 mg), $HfCl_4$ (40 mg) was dissolved in DMF (6 mL) and CH_3OH (6 mL). The mixture was transferred into a Parr Teflon–lined autoclave and kept at 130 °C for 72 h. After cooling down to room temperature, the colorless crystals were obtained and washed with CH_3OH. The crystals were achieved in a 38% yield based on TBC[8]. Elemental analysis (%): calculated for $[Hf_4Cl_2(H_2TBC[8])_2(HCOO)_2(CH_3OH)_4]\cdot 2CH_3OH\cdot 3DMF$, C 60.4, H 6.6, N 1.1; found, C 60.0, H 6.6, N 1.1.

Synthesis of Hf_8

A mixture of TBC[8] (100 mg), $HfCl_4$ (50 mg) was dissolved in DMF (5 mL), CH_3OH (5 mL) and en (1 mL). The mixture was transferred into a Parr Teflon–lined autoclave and kept at 130 °C for 72 h. After cooling down to room temperature, the colorless crystals were obtained and washed with CH_3OH. The crystals were achieved in a 40% yield based on TBC[8]. Elemental analysis (%): calculated for $[Hf_8(TBC[8])_2(C_3H_6NO_2)_2(\mu_4\text{-}O)_2(\mu_3\text{-}O)_2(\mu_3\text{-}OH)_4(\mu_2\text{-}OH)_2(H_2O)_4(CH_3OH)_2]\cdot 8CH_3OH\cdot 7DMF$, C 48.9, H 5.4, N 2.4; found, C 47.7, H 5.5, N 2.3.

Crystal data collection and refinements

All data collections were performed on a Bruker D8–Venture diffractometer with a Turbo X-ray Source (Cu Kα radiation, λ = 1.5418 Å) adopting the direct drive rotating anode technique and a CMOS detector at 293 K. The data frames were collected using the program APEX 3 and processed using the program SAINT routine in APEX 3. The structures were solved by direct methods and refined by the full matrix least-squares on F^2 using the SHELXL–2014 program. The diffused electron densities resulting from these residual solvent molecules were removed from the data set using the SQUEEZE routine of PLATON and refined further using the data generated. The restrained DFIX, SIMU, ISOR instructions were used to make the structures more reasonable. The formula unit was obtained through a combination of elemental analyses and

thermogravimetric characterization. CCDC number of 2322411-2322414 for **Zr4**, for **Hf4**, for **Zr8**, for **Hf_8**.

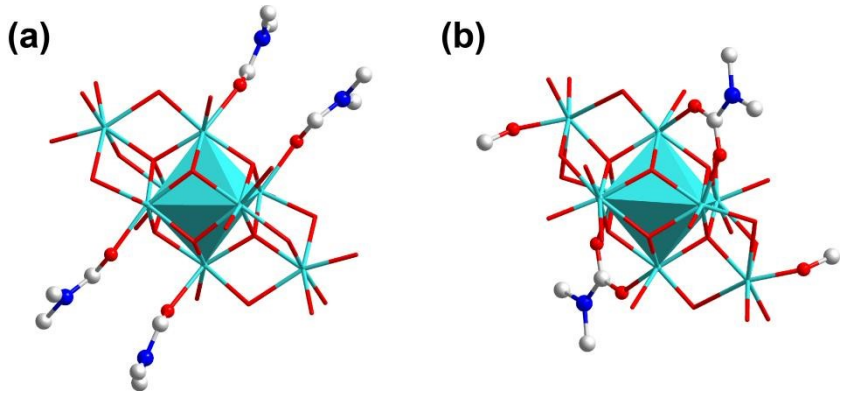

Fig. S1 Representation of **Zr_8** (a) and **Hf_8** (b) metallic core.

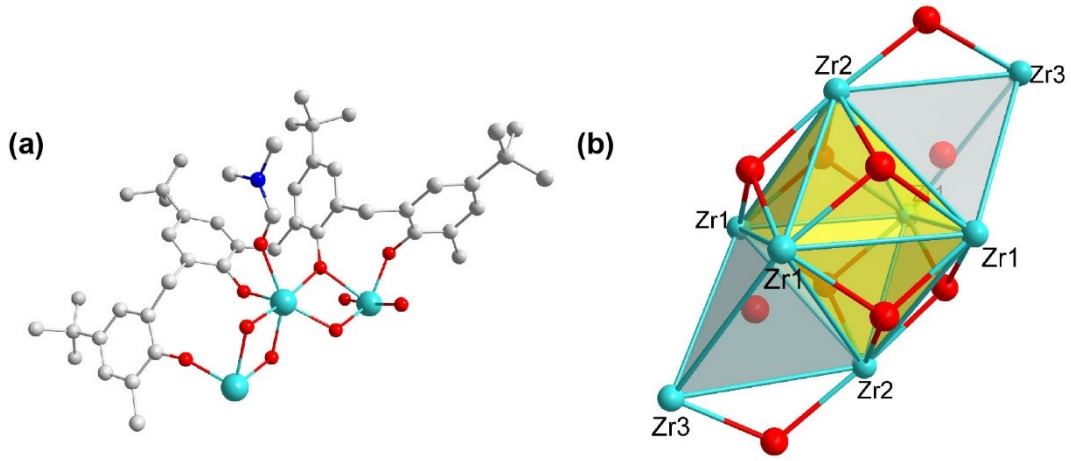

Fig. S2 (a) Asymmetric unit of **Zr_8**. (b) Representation of **Zr_8** metal core.

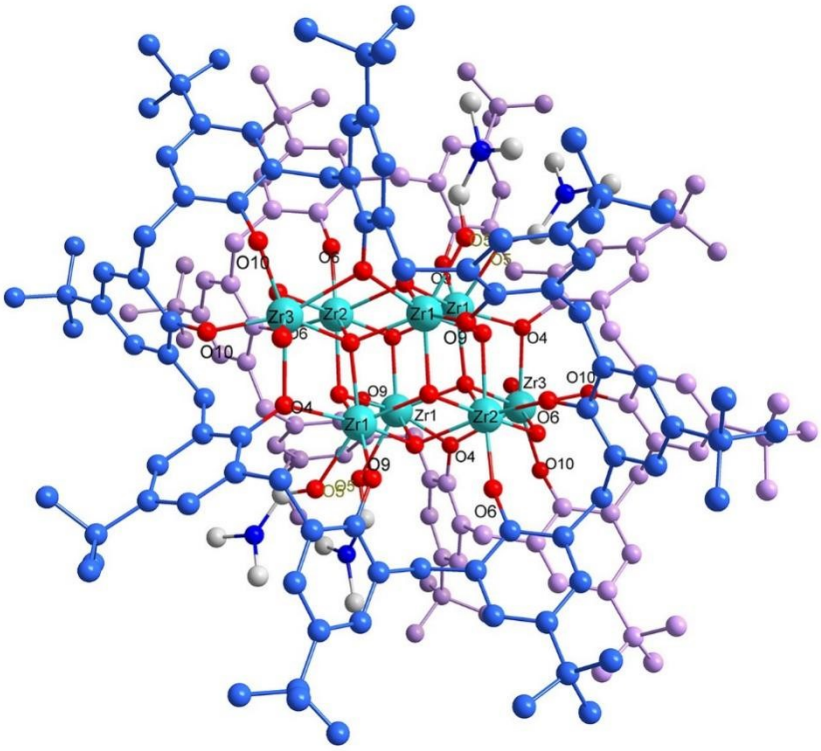

Fig. S3 Crystal structure of $\mathbf{Zr_8}$ with atomic labels.

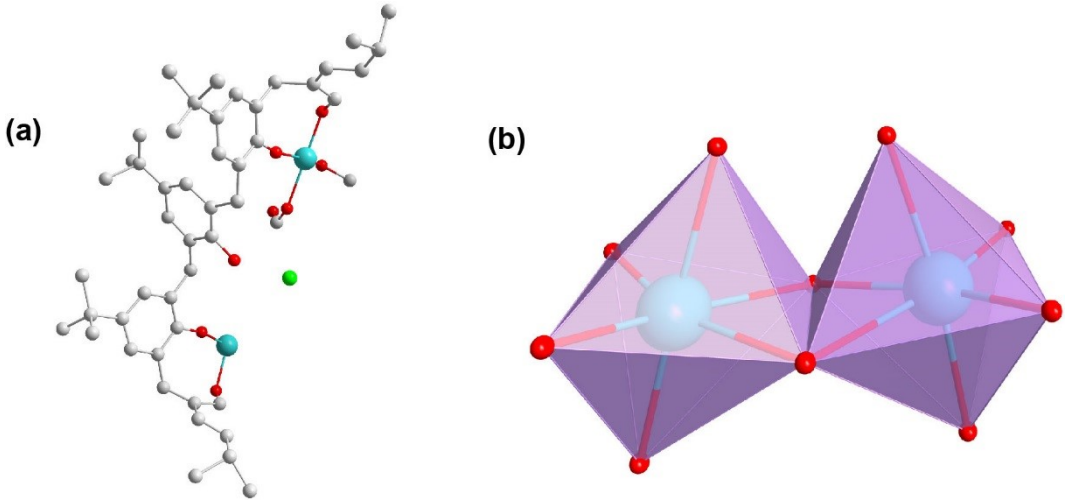

Fig. S4 (a) Asymmetric unit of $\mathbf{Zr_4}$. (b) Coordination mode of Zr in $\mathbf{Zr_4}$. All Zr sites are in the six-coordination environment.

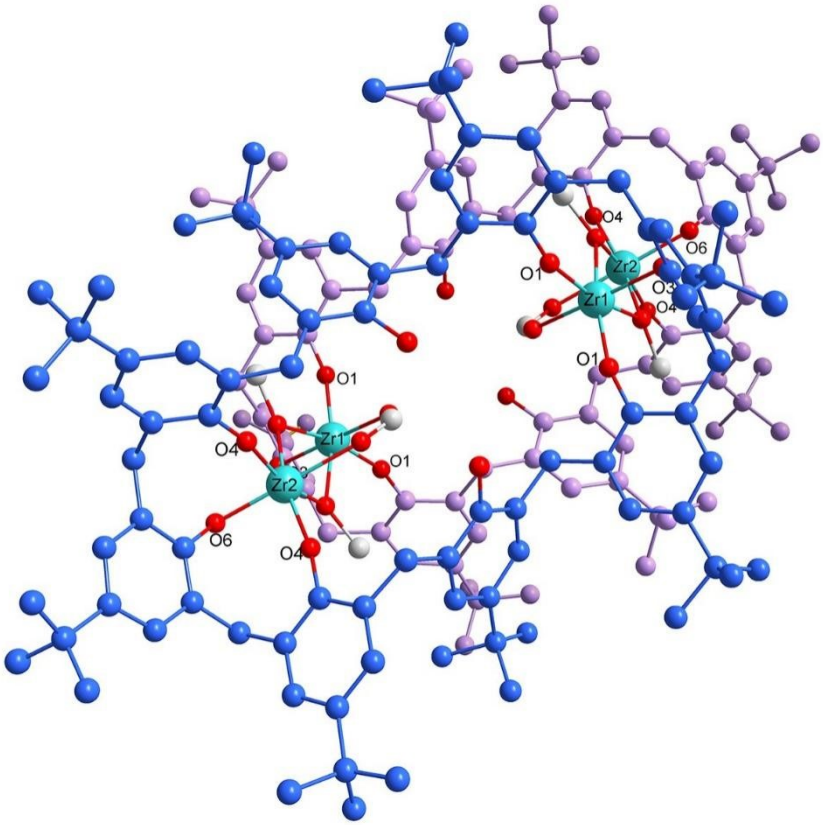

Fig. S5 Crystal structure of $\mathbf{Zr_4}$ with atomic labels.

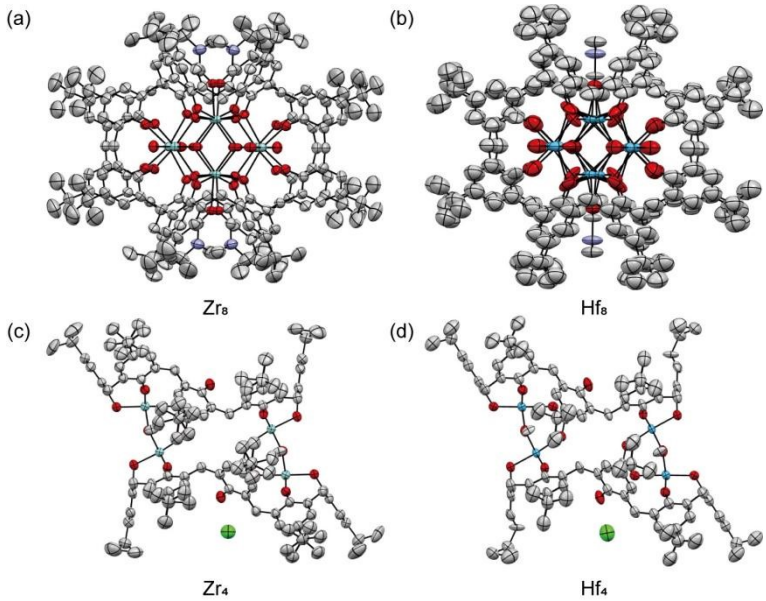

Fig. S6 Thermal ellipsoid plot drawings of the crystal structures of $\mathbf{Zr_8}$, $\mathbf{Hf_8}$, $\mathbf{Zr_4}$ and $\mathbf{Hf_4}$.

Table S1. The Crystallographic data for **Zr_4** and **Zr_8**

Compound	**Zr_4**	**Zr_8**
Empirical formula	$Zr_4Cl_2O_{29}C_{193}N_3H_{255}$	$Zr_8O_{47}N_{11}C_{217}H_{317}$
Formula weight	3516.89	4561.67
Crystal system	Monoclinic	Monoclinic
Space group	C2/m	C2/m
Temperature (K)	296.61	296.31
Wavelength (Å)	1.54178	1.54178
a (Å)	26.4909(13)	20.8087(15)
b (Å)	22.8712(12)	30.081(2)
c (Å)	19.5689(9)	18.0516(14)
α (°)	90	90
β (°)	122.050(3)	106.317(4)
γ (°)	90	90
Volume ($Å^3$)	10049.3(9)	10844.3(14)
Z	2	2
Dcalc. /mg·m-3	1.162	1.397
μ/mm^{-1}	2.338	3.502
F(000)	3408.0	3936.0
Limiting indices	-31<=h<=31, -27<=k<=27, -23<=l<=23	-24<=h<=24, -35<=k<=35, -19<=l<=21
Theta range for data collection (°)	5.328 to 133.696	8.184 to 134.368
Reflections collected	35632	46213
Independent reflections	8967 [R(int) = 0.0745]	9798 [R(int) = 0.0595]
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Data /restraints /	8967/601/603	9798/1110/549

parameters		
Goodness-of-fit on F2	1.039	1.052
Final R indices [I> 2sigma(I)]	R_1 = 0.0928, wR_2 = 0.2035	R_1 = 0.0766, wR_2 = 0.1883
R indices (all data)	R_1 = 0.1418, wR_2 = 0.2447	R_1 = 0.1025, wR_2 = 0.2161

Table S2. The Crystallographic data for **Hf_4** and **Hf_8**

Compound	**Hf_4**	**Hf_8**
Empirical formula	$Hf_4Cl_2O_{29}C_{193}N_3H_{255}$	$Hf_8O_{50}N_9C_{213}H_{307}$
Formula weight	3861.92	5221.66
Crystal system	Monoclinic	Monoclinic
Space group	C2/m	C2/m
Temperature (K)	290.56	290.56
Wavelength (Å)	0.71073	1.54178
a (Å)	26.560(8)	21.070(4)
b (Å)	22.889(6)	30.684(5)
c (Å)	19.280(6)	17.217(6)
α (°)	90	90
β (°)	120.746(10)	106.524(7)
γ (°)	90	90
Volume ($Å^3$)	10074(5)	10672(5)
Z	2	2
Dcalc. /mg·m-3	1.273	1.625
μ/mm^{-1}	2.122	7.415
F(000)	3630.0	4400.0
Limiting indices	-31<=h<=28, -26<=k<=27, -22<=l<=22	-24<=h<=24, -35<=k<=35, -20<=l<=19

Theta range for data collection (°)	4.94 to 50.222	5.354 to 128.872
Reflections collected	26987	55861
Independent reflections	9071 [R(int) = 0.0574]	8967 [R(int) = 0.0492]
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2
Data / restraints / parameters	9071/1066/ 516	8967/1229/526
Goodness-of-fit on F2	1.087	1.083
Final R indices [I > 2sigma(I)]	R_1 = 0.0854, wR_2 = 0.2197	R_1 = 0.1020, wR_2 = 0.2682
R indices (all data)	R_1 = 0.1370, wR_2 = 0.2798	R_1 = 0.1271, wR_2 = 0.2960

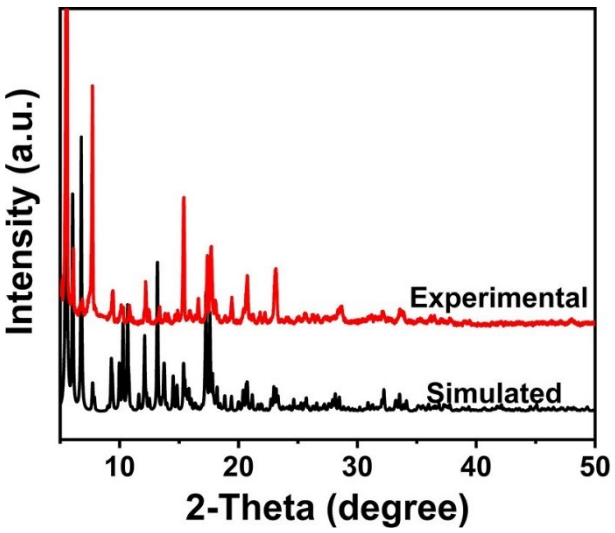

Fig. S7 Simulated and experimental PXRD pattern of **Zr_4**.

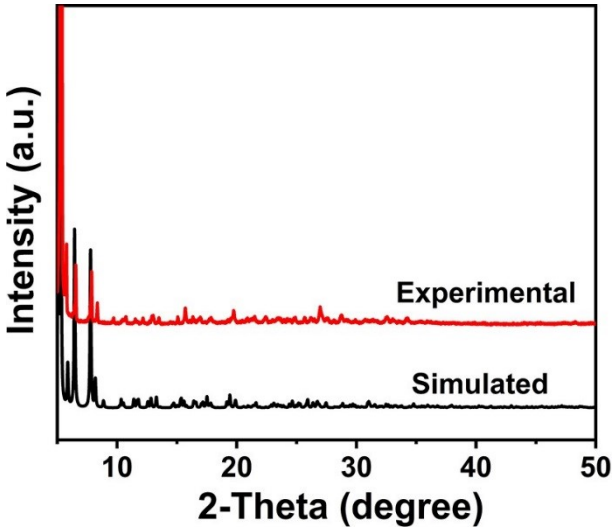

Fig. S8 Simulated and experimental PXRD pattern of $\mathbf{Zr_8}$.

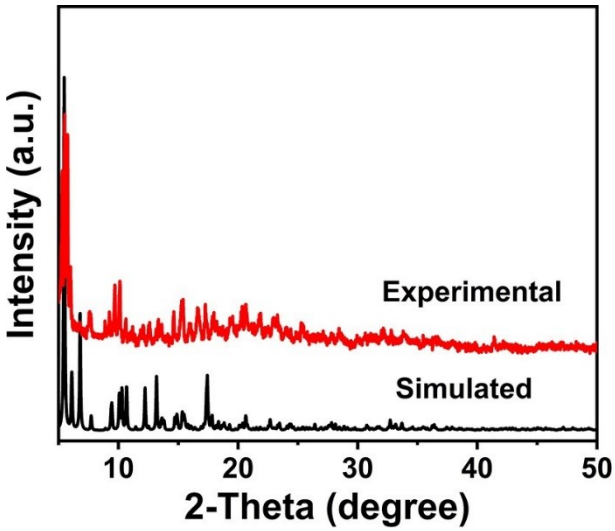

Fig. S9 Simulated and experimental PXRD pattern of $\mathbf{Hf_4}$.

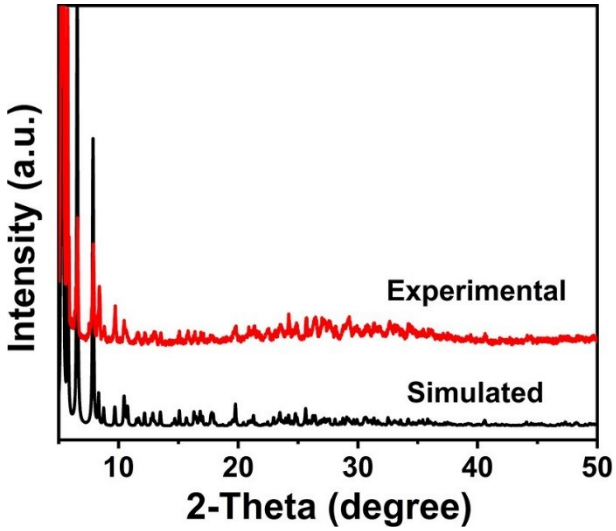

Fig. S10 Simulated and experimental PXRD pattern of $\mathbf{Hf_8}$.

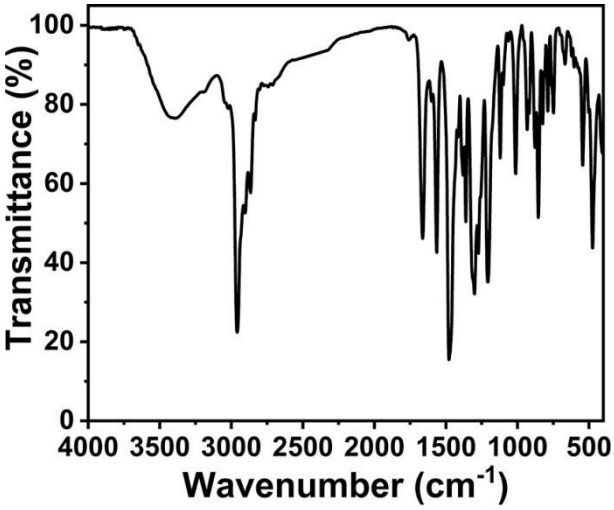

Fig. S11 IR curve of $\mathbf{Zr_4}$.

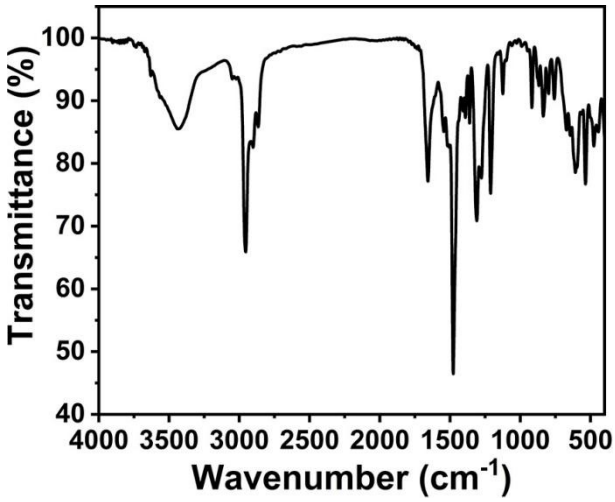

Fig. S12 IR curve of $\mathbf{Zr_8}$.

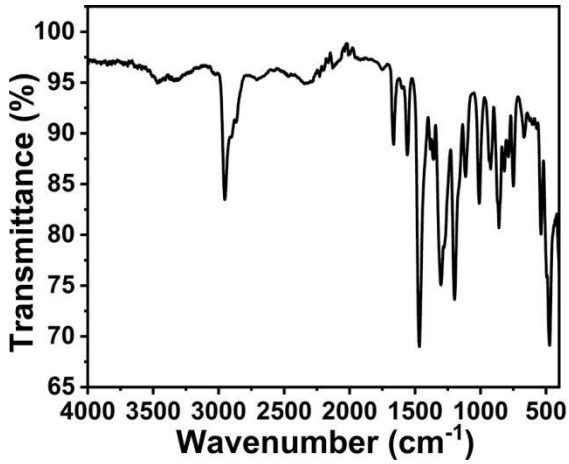

Fig. S13 IR curve of $\mathbf{Hf_4}$.

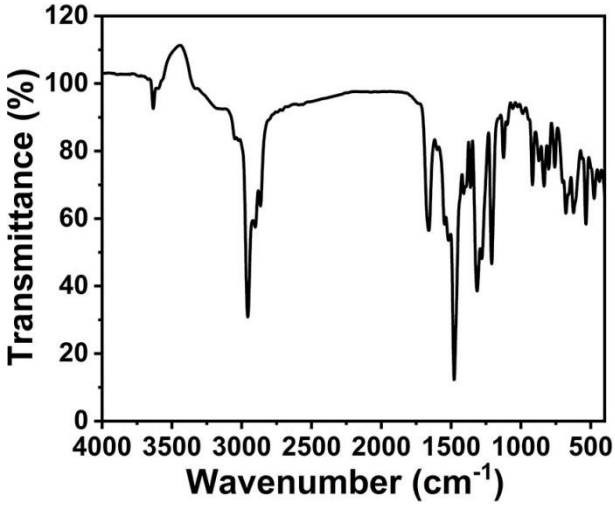

Fig. S14 IR curve of $\mathbf{Hf_8}$.

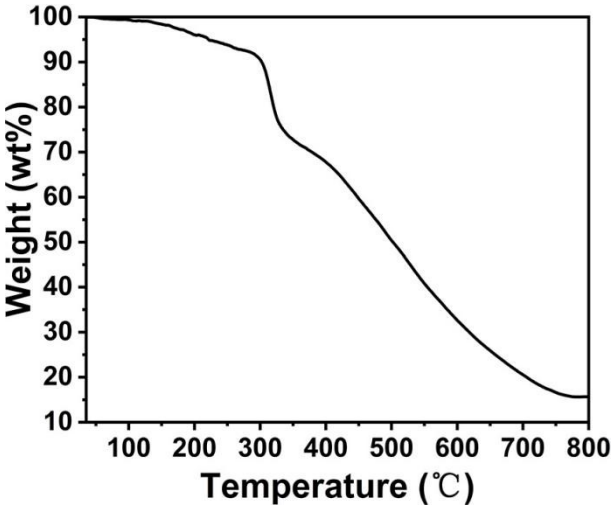

Fig. S15 TG curve of $\mathbf{Zr_4}$.

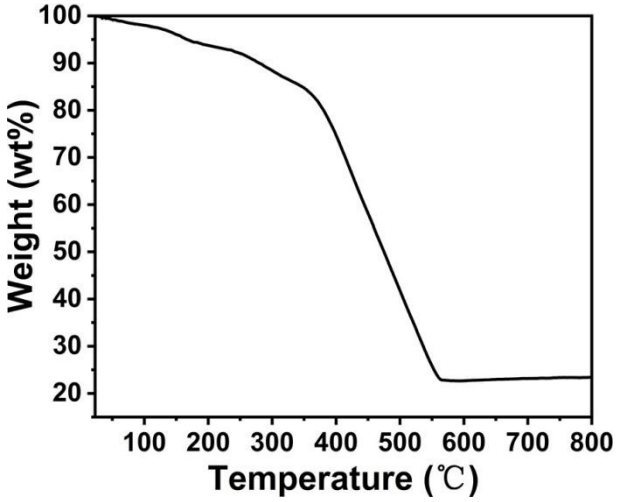

Fig. S16 TG curve of $\mathbf{Zr_8}$.

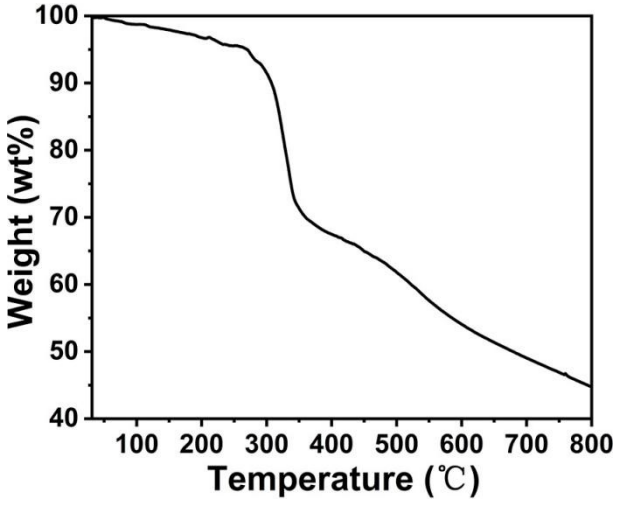

Fig. S17 TG curve of **Hf_4**.

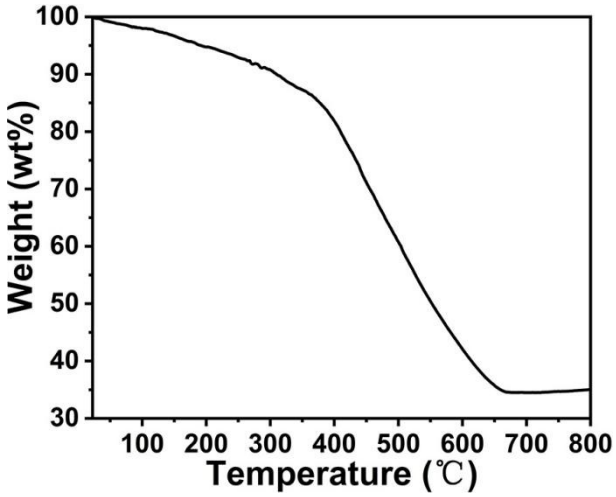

Fig. S18 TG curve of **Hf_8**.

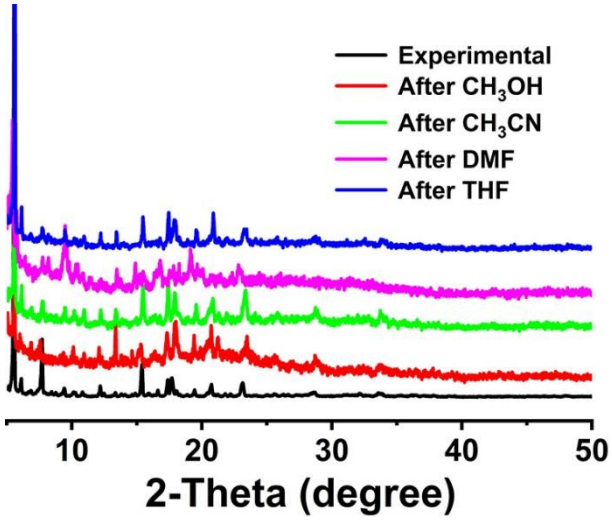

Fig. S19 Stability tests of **Zr_4** in different solvent.

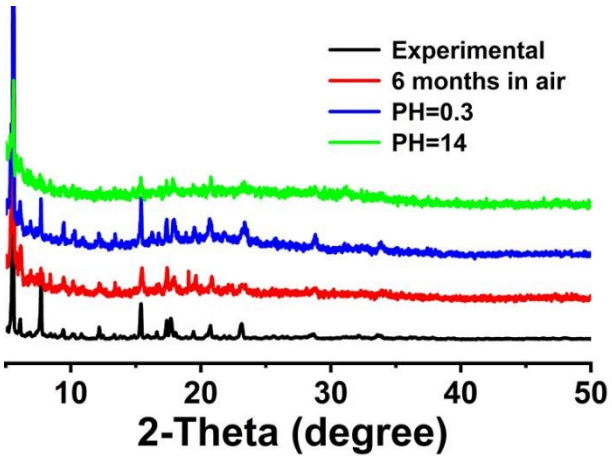

Fig. S20 Stability tests of $\mathbf{Zr_4}$ in air and aqueous solutions with different pH values.

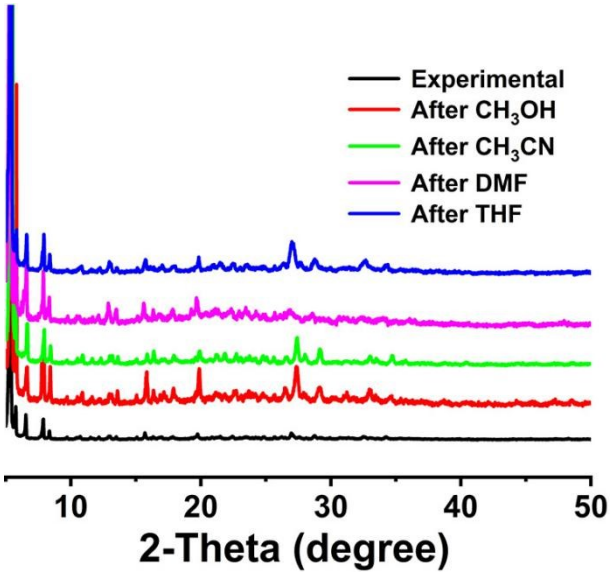

Fig. S21 Stability tests of $\mathbf{Zr_8}$ in different solvent.

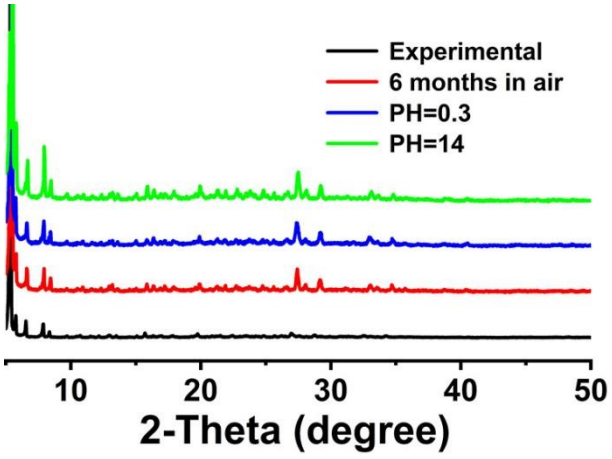

Fig. S22 Stability tests of $\mathbf{Zr_8}$ in air and aqueous solutions with different pH values.

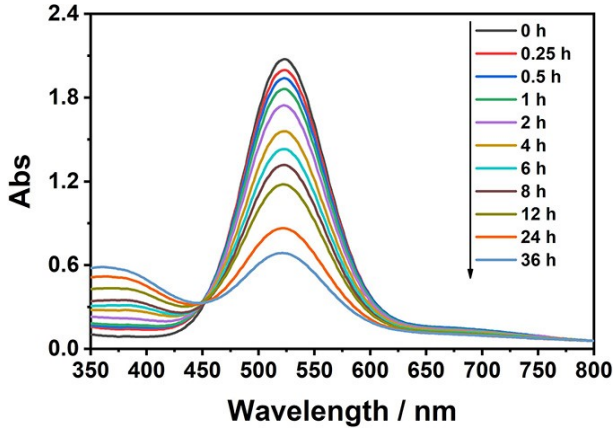

Fig. S23 Temporal evolution of UV−vis absorption spectra of **Hf_4** captured by I_2 in an iodine/cyclohexane solution (2×10^{-3} mol L−1).

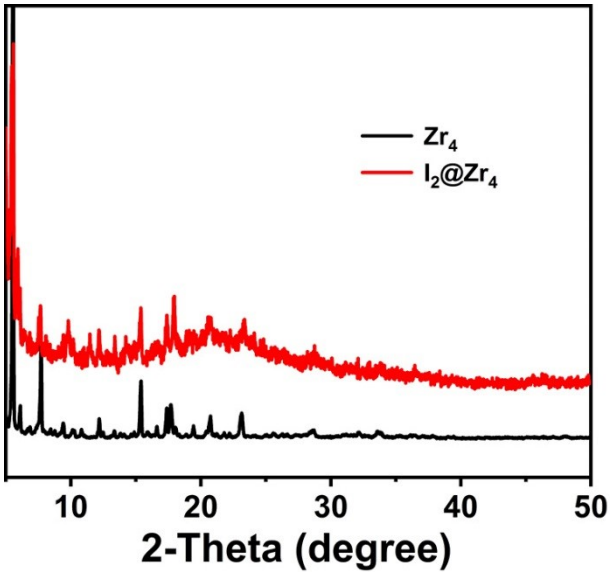

Fig. S24 PXRD pattern of **Zr_4** and **I_2@Zr_4**.

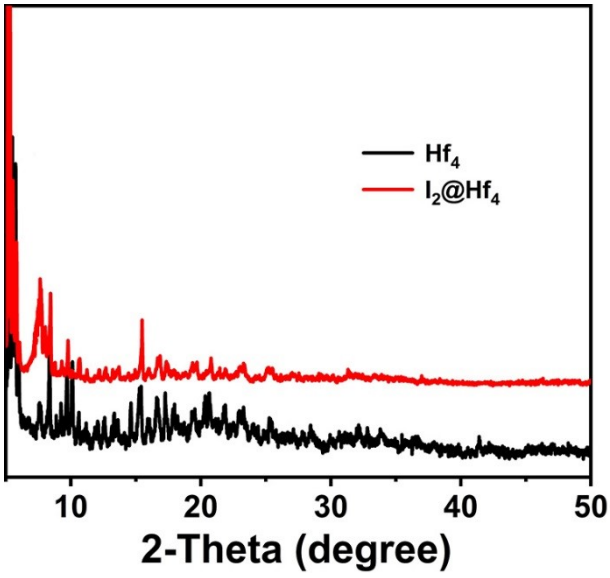

Fig. S25 PXRD pattern of **Hf_4** and **I_2@Hf_4**.

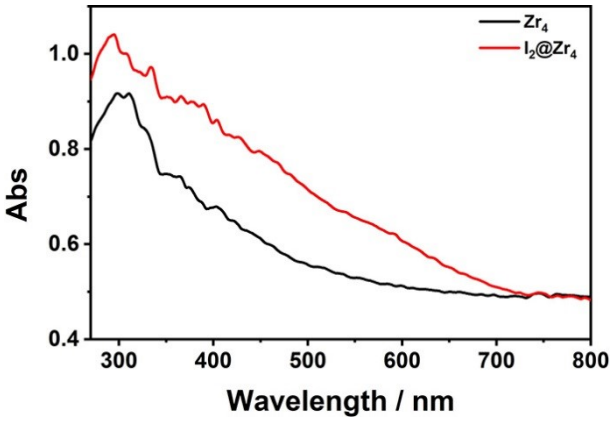

Fig. S26 Solid UV/visible absorption spectra of **Zr_4** and **I_2@Zr_4**.

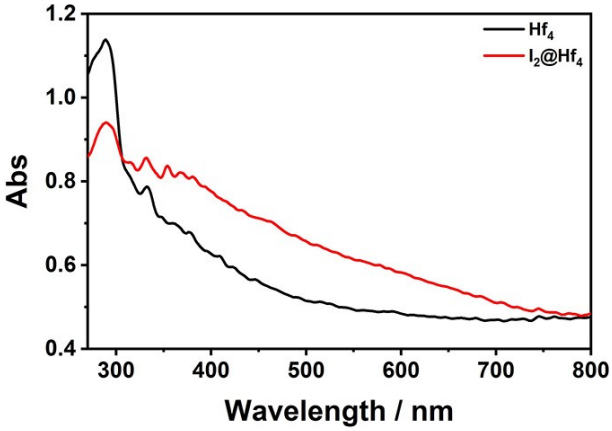

Fig. S27 Solid UV/visible absorption spectra of **Hf_4** and **I_2@Hf_4**.

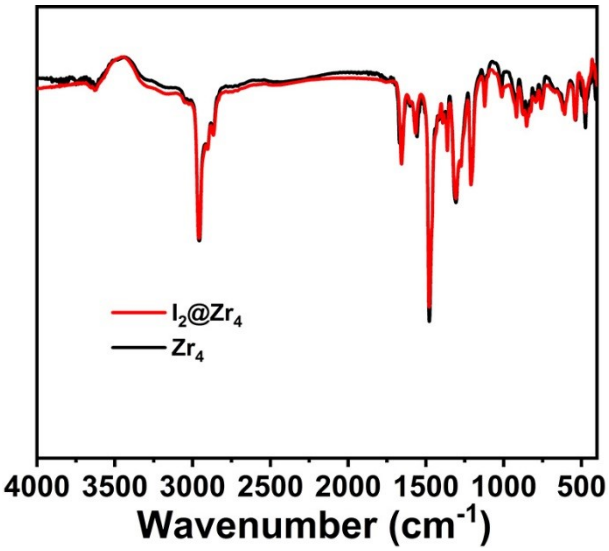

Fig. S28 FT-IR spectra of $\mathbf{Zr_4}$ and $\mathbf{I_2@Zr_4}$.

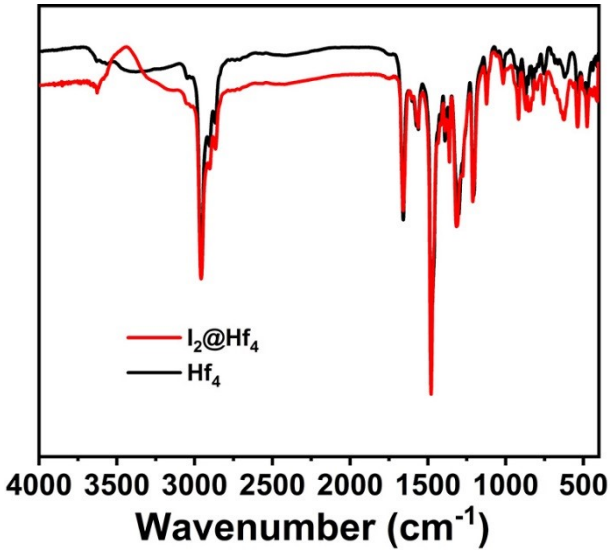

Fig. S29 FT-IR spectra of $\mathbf{Hf_4}$ and $\mathbf{I_2@Hf_4}$.

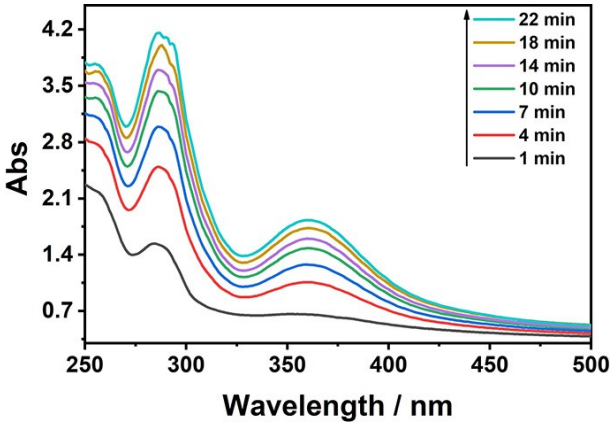

Fig. S30 UV-Vis absorption spectra of iodine released from $\mathbf{I_2@Hf_4}$ with 3 ml of acetonitrile.

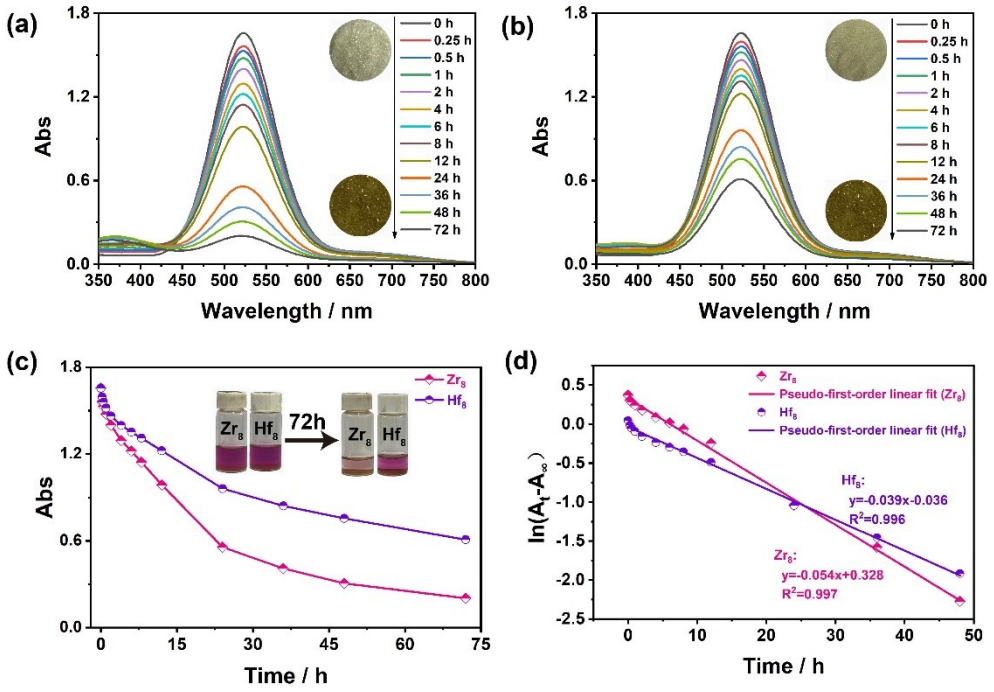

Fig. S31 Temporal evolution of UV−Vis absorption spectra of (a) $\mathbf{Zr_8}$ and (b) $\mathbf{Hf_8}$ captured by I_2 in an iodine/cyclohexane solution (2×10^{-3} mol L^{-1}). (c) Plots of time vs absorbance for $\mathbf{Zr_8}$ and $\mathbf{Hf_8}$ monitored at 523 nm of iodine at selected time intervals. (d) Kinetic analysis of $\mathbf{Zr_8}$ and $\mathbf{Hf_8}$ monitored at 523 nm of iodine adsorption at different time intervals.

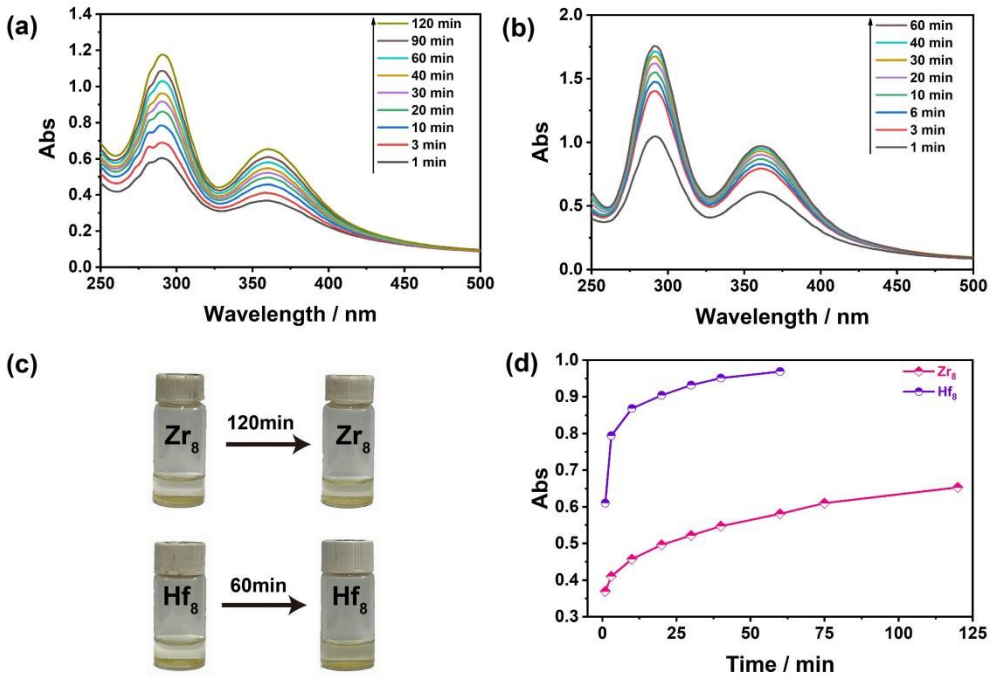

Fig. S32 UV-Vis absorption spectra of iodine released from (a) $\mathbf{I_2@Zr_8}$ and (b) $\mathbf{I_2@Hf_8}$ with 3 ml of acetonitrile. (c) Photographs of the color change of acetonitrile solutions of samples $\mathbf{I_2@Zr_8}$ and $\mathbf{I_2@Hf_8}$ after iodine release. (d) Plots of time vs absorbance for $\mathbf{I_2@Zr_8}$ and $\mathbf{I_2@Hf_8}$ monitored at different time intervals, respectively.

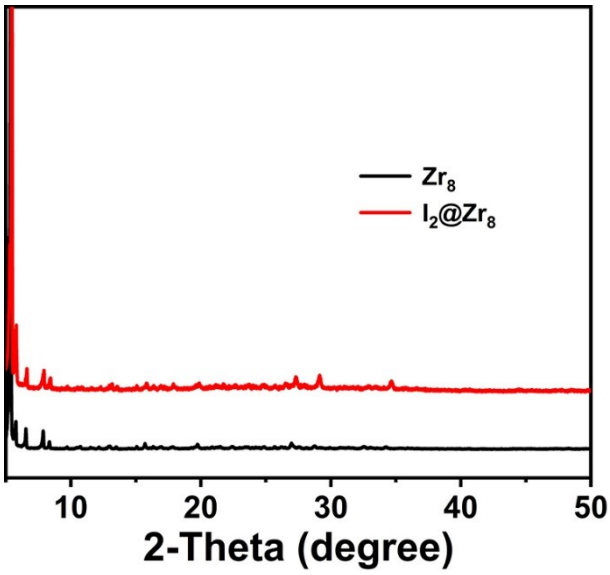

Fig. S33 PXRD pattern of $\mathbf{Zr_8}$ and $\mathbf{I_2@Zr_8}$.

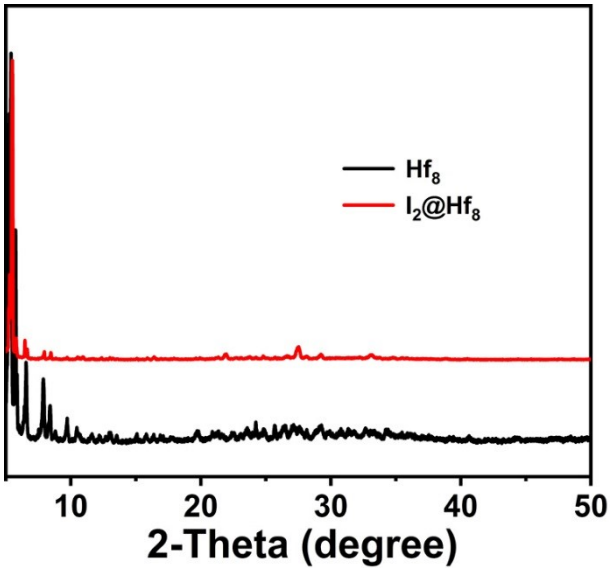

Fig. S34 PXRD pattern of **Hf_8** and **I_2@Hf_8**.

Table 3. Cartesian coordinates of **Zr_4** model complex used in DFT calculation

Symbol	x/a	y/b	z/c	Symbol	x/a	y/b	z/c
Zr1	0.54977	0.50563	0.71651	O136	0.68977	0.50581	0.66029
Zr2	0.6763	0.50497	0.75141	O137	0.66276	0.50457	0.84237
O3	0.48823	0.44333	0.69044	C138	0.47612	0.62643	0.69619
O4	0.48879	0.56857	0.69066	C139	0.62323	0.60378	0.69378
O5	0.61137	0.56916	0.74185	C140	0.6243	0.40187	0.69798
O6	0.61077	0.44141	0.74158	Zr141	0.6219	0.50564	0.39612
O7	0.51438	0.50565	0.8013	O142	0.68376	0.44125	0.41819
H8	0.44056	0.19439	0.62221	O143	0.68273	0.57136	0.41697
Zr9	0.49063	0.50432	0.36534	O144	0.65221	0.50504	0.30929
Zr10	0.62192	0.5056	0.39609	C145	0.54992	0.40425	0.42076
O11	0.55969	0.44202	0.37459	C146	0.39137	0.61894	0.33639
O12	0.55868	0.56786	0.37361	C147	0.45285	0.61316	0.79963
O13	0.42652	0.57455	0.35574	C148	0.42418	0.6121	0.23122
O14	0.42262	0.4372	0.35961	H149	0.33592	0.59645	0.15821
O15	0.4888	0.49849	0.45758	H150	0.33822	0.59717	0.80311
O16	0.4778	0.50081	0.26947	H151	0.23957	0.56207	0.17428
C17	0.47653	0.38526	0.69534	H152	0.27453	0.59059	0.11507
C18	0.54838	0.60615	0.41919	H153	0.20918	0.55581	0.10657

C19	0.4541	0.50521	0.79715	H154	0.24357	0.6181	0.83837
C20	0.38904	0.39211	0.33886	H155	0.19334	0.55141	0.86975
C21	0.53317	0.50684	0.49773	H156	0.2775	0.56261	0.89094
C22	0.43033	0.5048	0.22685	H157	0.22516	0.50502	0.73327
O23	0.59196	0.5064	0.48316	H158	0.18224	0.56771	0.76814
O24	0.40364	0.43038	0.53925	H159	0.2673	0.58088	0.74471
H25	0.37928	0.45097	0.50835	C160	0.64463	0.49202	0.62182
C26	0.42762	0.38018	0.51567	C161	0.45141	0.64777	0.74817
C27	0.45211	0.36322	0.74712	C162	0.4783	0.66054	0.64542
C28	0.4787	0.35181	0.64417	H163	0.6291	0.57711	0.65726
C29	0.47677	0.35385	0.54211	H164	0.66107	0.62821	0.70075
C30	0.40348	0.35545	0.46456	H165	0.58806	0.63189	0.68646
C31	0.42359	0.45114	0.79681	H166	0.63308	0.42371	0.65904
C32	0.45413	0.39716	0.79898	H167	0.66095	0.37773	0.71039
C33	0.36217	0.45108	0.80094	H168	0.58894	0.37374	0.69176
C34	0.42289	0.55884	0.79695	H169	0.5387	0.42811	0.45796
C35	0.50153	0.37775	0.59306	H170	0.51595	0.37567	0.41029
C36	0.50401	0.30574	0.51528	H171	0.58788	0.38035	0.42898
C37	0.3874	0.37699	0.27902	C172	0.38797	0.63356	0.27664
C38	0.34863	0.3319	0.27573	C173	0.35432	0.6491	0.37818
C39	0.42474	0.39807	0.2343	H174	0.43453	0.63768	0.83343
C40	0.35187	0.36113	0.37985	H175	0.49645	0.60478	0.81005
C41	0.43116	0.30765	0.43753	H176	0.42552	0.64262	0.19736
C42	0.35323	0.37974	0.43862	H177	0.46627	0.6061	0.2477
H43	0.54665	0.37124	0.59203	H178	0.65541	0.47194	0.58232
H44	0.49308	0.42256	0.59418	C179	0.4255	0.70384	0.748
C45	0.3124	0.3141	0.3639	C180	0.50136	0.63523	0.59408
H46	0.43638	0.37222	0.83278	C181	0.45186	0.71595	0.64481
H47	0.4978	0.40581	0.80888	C182	0.34861	0.67803	0.27411
C48	0.404	0.45125	0.21051	C183	0.35618	0.62983	0.43673
C49	0.40363	0.55799	0.20942	C184	0.31381	0.69553	0.36318
H50	0.41438	0.29051	0.39874	H185	0.40678	0.72052	0.78609
C51	0.48123	0.28272	0.46309	C186	0.42407	0.7369	0.69567
C52	0.42536	0.30758	0.7461	C187	0.47713	0.65849	0.54254
H53	0.33952	0.41153	0.80262	H188	0.54644	0.64206	0.59344

C54	0.33141	0.50429	0.80491	H189	0.4934	0.59033	0.59511
C55	0.50873	0.23469	0.4365	H190	0.45176	0.74093	0.60665
C56	0.45168	0.29671	0.64274	C191	0.31069	0.71269	0.30421
C57	0.35527	0.45069	0.17288	C192	0.40568	0.6549	0.46332
H58	0.54119	0.28719	0.53405	H193	0.35995	0.58442	0.43793
C59	0.33049	0.50363	0.15376	H194	0.31833	0.6428	0.4586
C60	0.35491	0.55722	0.17166	C195	0.39573	0.79148	0.6939
C61	0.27792	0.50291	0.12171	C196	0.4285	0.63159	0.51569
H62	0.35566	0.42524	0.44049	C197	0.5049	0.70602	0.51521
H63	0.31583	0.36529	0.46032	C198	0.27552	0.75789	0.28193
H64	0.52181	0.51244	0.54155	C199	0.43395	0.70207	0.43581
C65	0.31046	0.29669	0.30494	C200	0.33474	0.78296	0.69415
H66	0.42767	0.36687	0.20117	C201	0.41241	0.82554	0.74238
H67	0.46623	0.40514	0.25187	C202	0.41194	0.81988	0.64169
H68	0.2864	0.29363	0.39527	O203	0.40406	0.58194	0.53997
H69	0.3365	0.41102	0.16051	C204	0.48352	0.72749	0.46176
H70	0.53735	0.58264	0.45666	H205	0.54159	0.7251	0.53441
H71	0.51407	0.63412	0.4082	C206	0.2353	0.78409	0.33573
H72	0.58603	0.63065	0.42712	C207	0.31732	0.81066	0.25633
C73	0.2764	0.25089	0.28202	C208	0.2385	0.73677	0.23761
H74	0.4512	0.27236	0.60418	H209	0.41809	0.71824	0.39624
C75	0.42344	0.27545	0.69323	H210	0.32264	0.76142	0.73248
H76	0.40623	0.29064	0.78387	H211	0.31375	0.82339	0.69208
C77	0.39206	0.22266	0.68989	H212	0.32278	0.75774	0.65809
C78	0.36144	0.55798	0.80119	H213	0.45758	0.83171	0.74172
C79	0.27097	0.50378	0.81652	H214	0.39146	0.86599	0.7404
C80	0.24392	0.22653	0.32835	H215	0.40053	0.80402	0.78079
C81	0.31958	0.20035	0.25411	H216	0.3911	0.86035	0.63914
C82	0.23785	0.27232	0.23906	H217	0.45713	0.82588	0.64119
C83	0.24836	0.55632	0.12991	H218	0.3811	0.56008	0.50887
C84	0.24276	0.4567	0.14231	C219	0.51163	0.77469	0.43434
C85	0.28973	0.49456	0.06186	H220	0.28356	0.79754	0.36209
C86	0.56841	0.24753	0.42848	H221	0.204	0.80356	0.37955
C87	0.48192	0.22351	0.38223	H222	0.35077	0.85244	0.23603
C88	0.50274	0.18591	0.47359	H223	0.27022	0.83934	0.24373

C89	0.33281	0.23313	0.70302	H224	0.33984	0.81519	0.30804
C90	0.41542	0.18171	0.72944	H225	0.2118	0.70381	0.25437
C91	0.39667	0.20136	0.63226	H226	0.21259	0.7711	0.22247
C92	0.24756	0.45173	0.83967	H227	0.26355	0.72023	0.20329
C93	0.24288	0.56306	0.84709	H228	0.33823	0.77334	0.21931
C94	0.23325	0.54546	0.77096	H229	0.21235	0.73261	0.34025
H95	0.32936	0.24959	0.7454	C230	0.53044	0.75739	0.37831
H96	0.30943	0.19412	0.69984	C231	0.55995	0.79138	0.46865
H97	0.31584	0.26347	0.6735	C232	0.47174	0.82137	0.42972
H98	0.25407	0.41766	0.81008	H233	0.49438	0.74448	0.35356
H99	0.20291	0.4571	0.84721	H234	0.55132	0.79235	0.3578
H100	0.26854	0.44192	0.87895	H235	0.55947	0.72243	0.38224
H101	0.23393	0.46292	0.18661	H236	0.58879	0.75625	0.47228
H102	0.2648	0.41718	0.13664	H237	0.58117	0.82664	0.44902
H103	0.20359	0.45581	0.11898	H238	0.54549	0.80342	0.51019
H104	0.31153	0.45493	0.0561	H239	0.49206	0.85689	0.4096
H105	0.31584	0.52869	0.04659	H240	0.43586	0.80821	0.40485
H106	0.25049	0.49385	0.03864	H241	0.45771	0.83343	0.4714
H107	0.27249	0.211	0.36031	H242	0.52304	0.14975	0.45466
H108	0.21844	0.19214	0.31263	H243	0.39971	0.79411	0.6061
H109	0.21692	0.25853	0.34642	H244	0.21271	0.82127	0.29957
H110	0.45929	0.17429	0.71948	C245	0.7158	0.62141	0.77944
H111	0.39222	0.14259	0.72632	C246	0.72004	0.3972	0.79861
H112	0.41201	0.19832	0.77183	C247	0.71639	0.50428	0.87013
H113	0.44284	0.18446	0.59431	C248	0.67505	0.39258	0.38357
H114	0.57256	0.28412	0.40159	C249	0.67393	0.61878	0.38074
H115	0.58923	0.21188	0.40913	C250	0.71196	0.51377	0.30988
H116	0.58748	0.25622	0.46899	H251	0.68544	0.63543	0.74852
H117	0.35387	0.16021	0.23197	H252	0.69481	0.61495	0.8194
H118	0.27325	0.17043	0.24153	H253	0.74822	0.65312	0.78422
H119	0.34341	0.19528	0.30516	H254	0.73987	0.5415	0.85812
H120	0.21071	0.30399	0.25751	H255	0.71016	0.50407	0.9153
H121	0.21246	0.23798	0.22309	H256	0.73959	0.46702	0.85775
H122	0.26179	0.29077	0.20492	H257	0.75151	0.36453	0.80329
H123	0.43767	0.21467	0.38878	H258	0.68161	0.37912	0.78199

H124	0.50194	0.18765	0.36242	H259	0.71163	0.41623	0.8392
H125	0.48625	0.26018	0.35547	H260	0.63151	0.63456	0.38636
H126	0.52223	0.19508	0.51379	H261	0.67981	0.60576	0.33743
H127	0.45845	0.17704	0.47988	H262	0.70394	0.65152	0.39109
H128	0.33867	0.2394	0.21791	H263	0.72103	0.55396	0.32945
H129	0.42673	0.22368	0.77364	H264	0.72786	0.51363	0.26715
H130	0.3793	0.23209	0.60338	H265	0.73191	0.48041	0.33374
H131	0.37363	0.16219	0.62853	H266	0.68017	0.40422	0.33978
Zr132	0.67635	0.50496	0.75143	H267	0.6329	0.37649	0.39022
O133	0.58632	0.50539	0.63219	H268	0.70555	0.36049	0.39449
O134	0.74024	0.43949	0.76054	I269	0.39453	0.50521	0.30753
O135	0.741	0.5696	0.76133	I270	0.29915	0.50946	0.36393