Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Co-crystal of Ti_4Ni_2 and Ti_8Ni_4 clusters with enhanced photochemical properties

Chao Wang*, Yong Jun Lu, Ming Yang Rao, Ning Chen, Shou Juan Wang, Fan Gong Kong*

State Key Laboratory of Biobased Material and Green Papermaking, Qilu University of Technology, Shandong Academy of Sciences, Jinan, 250353, China,
E-mail: wangchao@qlu.edu.cn.

1. Experimental section

Materials, Syntheses and Characterization. All reagents were purchased from Aladdin and without further purified before utilization. A UV-vis spectrum (200-800 nm) was obtained on an UV-4000 spectrophotometer. A VarioEL analyzer was used to analyze the elemental composition of compounds. A Bruker D_8 Focus diffractometer was used to record the powder X-ray diffraction (XRD) data of compounds (Cu-Kα, λ=1.5405 nm). The Fourier transform infrared (FTIR) spectra were obtained on a Nicolet 7600 spectrometer (500-4000 cm^{-1}). The thermogravimetric analysis (TGA) experiments were performed from 50 to 800 °C (10 °C·min^{-1}, N_2). We collected crystallographic data on an Agilent Gemini E dual-light source X-ray single crystal diffractometer with Eos CCD detector. The CCDC numbers of **1** and **2** are 2052629 and 2052630, and the specific crystallographic information can be received from the Cambridge Crystallographic Data Centre.

Photocurrent Measurement. Each electrode for photocurrent test was prepared through a solution spin coating. Typically, fresh sample (5 mg) was directly dispersed to dichloromethane (1 mL), and then the dispersion solution was coated onto 1 cm^2 of pre-cleaned indium tin oxide (ITO) glass. The testing electrode was obtained after evaporation at room atmosphere. A xenon lamp (300 W) coupled with cut-off filter was used for the photocurrent measurements. Photocurrent measurements were performed on an electrochemical workstation (CHI650) with a standard three-electrode system. The prepared electrode, a platinum plate and a saturated Ag/AgCl (3 M KCl) electrode were adopted as the working, counter and reference electrodes, respectively. A 0.2 M solution of $NaSO_4$ was employed as the electrolyte.

Hydrogen Production Experiment. Hydrogen production experiment was investigated in a closed gas circulation system. Typically, the fresh sample (50 mg) was dispersed into the mixed solution embodying water (90 mL) and methanol (10 mL, as sacrificial agent), followed by the addition of 1.0 wt% $HPtCl_4$ (33 μL). The visible light irradiation was provided by a 300 W Xe lamp. Before reaction, the reaction system was evacuated to completely remove the dissolved oxygen in the solution by aeration of Ar gas. After turning on the Xe lamp, the hydrogen evolution reaction was kept for 4 h. The amount of hydrogen evolution was monitored by online gas chromatography (GC) analysis system at interval of 1 hour.

Single-crystal structure determinations. Crystallographic data were collected an Agilent Gemini E dual-light source X-ray single crystal diffractometer with Eos CCD detector. The structures are solved by the inherent phase method in the SHELXT [1] program, and refined by the least square method in the SHELXL[1] program. Both programs are used coupling with OLEX2.[2] All non-hydrogen atoms, including free solvent and host molecules, are directly identified by the SHELXT program and refined

by anisotropically. Crystallographic data for compounds **1** and **2** are summarized in **Table S1** in the Supporting Information.

Computational Methods. All calculations were done using the Gaussian 09 program.[3] Geometry optimization calculations for the two sub-clusters of cluster **2** were performed by using the B3LYP DFT method on the basis of the crystal structures. The basis set used for the C, H, O and N atoms was 6-31G*, and the LANL2DZ pseudopotential basis set was employed for Ti and Ni atoms.

2. Crystallographic details

Table S1 X-ray measurements and structure solution of clusters **1** and **2**.

Compound	**1**	**2**
Empirical formula	$C_{82}H_{67}NNi_2O_{28}Ti_4$	$C_{226}H_{193}N_7Ni_6O_{78}Ti_{12}$
Formula weight	1823.23	5181.46
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a (Å)	14.4874	13.2237
b (Å)	14.5800	15.5692
c (Å)	22.5228	30.2206
α (°)	103.963	78.592
β (°)	91.480	79.32
γ (°)	116.861	71.855
V	4068.4	5744.40
Z	2	1
ρ_{calc} ($g \cdot cm^{-3}$)	1.488	1.498
μ (mm^{-1})	0.909	4.608
F(000)	1868.0	2654.0
Data/restraints/ parameters	16593/0/1059	23107/27/1505
R_1/wR_2 ($I>2\sigma(I)$)[a]	0.0557/0.1464	0.0485/0.1356
R_1/wR_2 (all data)[a]	0.0934/0.1753	0.0527/0.1401
GooF (all data)[b]	1.008	1.066

[a]$R_1=\sum||Fo|-|Fc||/\sum|Fo|$; $wR_2=\{\sum w[(Fo)^2-(Fc)^2]^2/\sum w[(Fo)^2]^2\}^{1/2}$

[b]$GooF=\{\sum w[(Fo)^2-(Fc)^2]^2/(n-p)\}^{1/2}$

3. Crystal structures

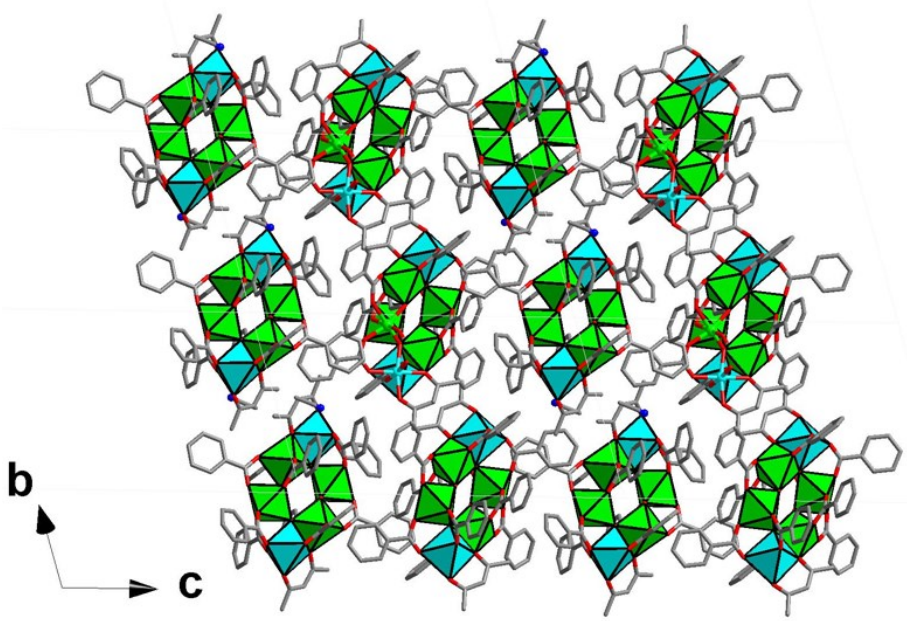

Figure S1 Packing structure of cluster **1** along the *a*-axis.

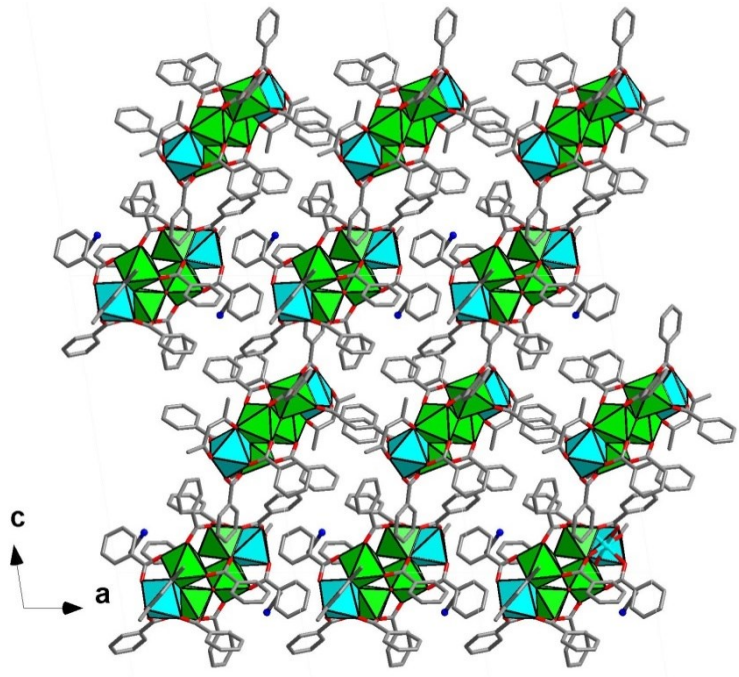

Figure S2 Packing structure of cluster **1** along the *b*-axis.

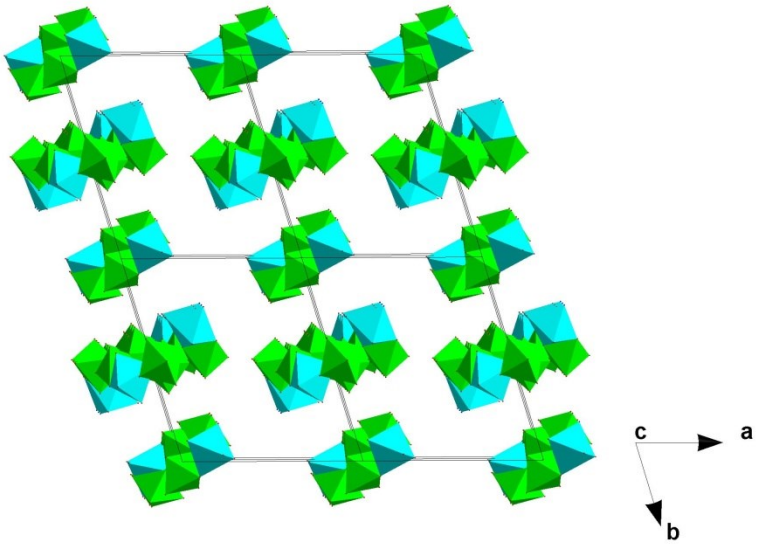

Figure S3 Packing structure of cluster **2** along the *c*-axis.

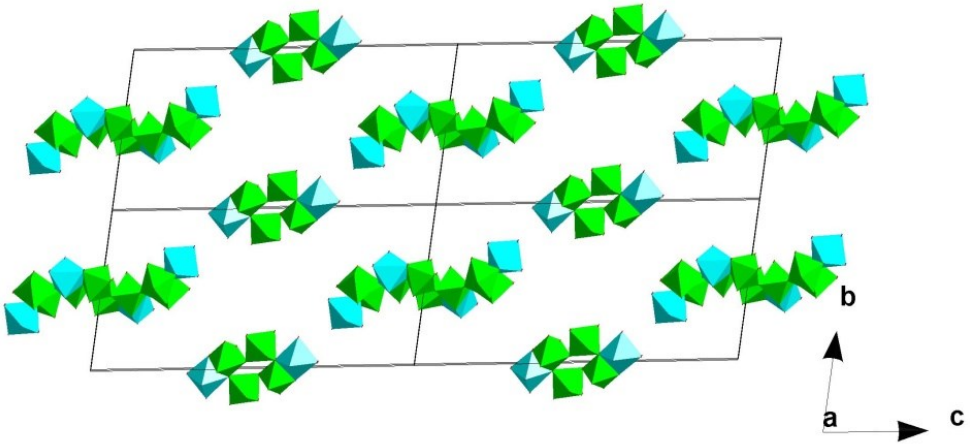

Figure S4 Packing structure of cluster **2** along the *a*-axis.

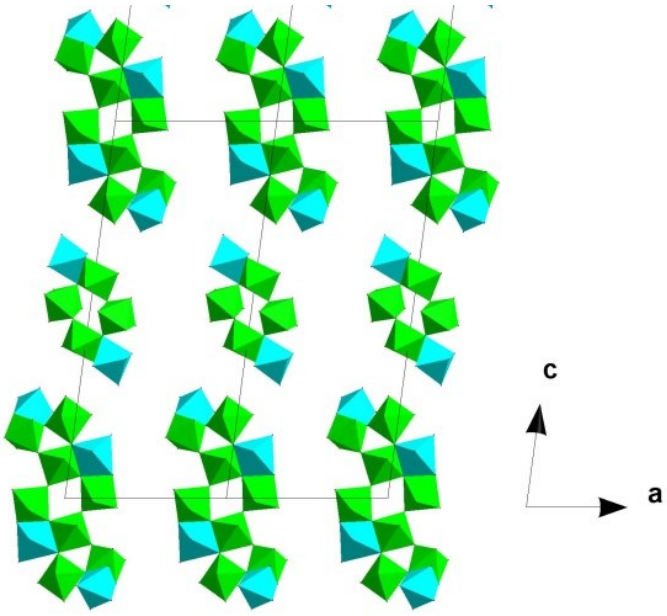

Figure S5 Packing structure of cluster **2** along the *b*-axis.

4. Powder X-ray diffraction

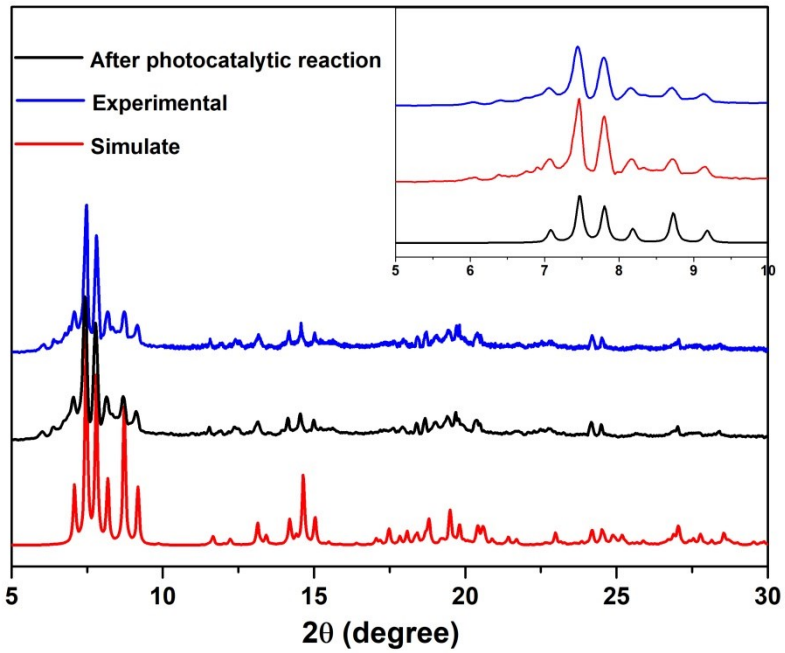

Figure S6 The XRD patterns of cluster 1 (the simulated pattern, as-synthesized product and sample 1 after photocatalytic experiment).

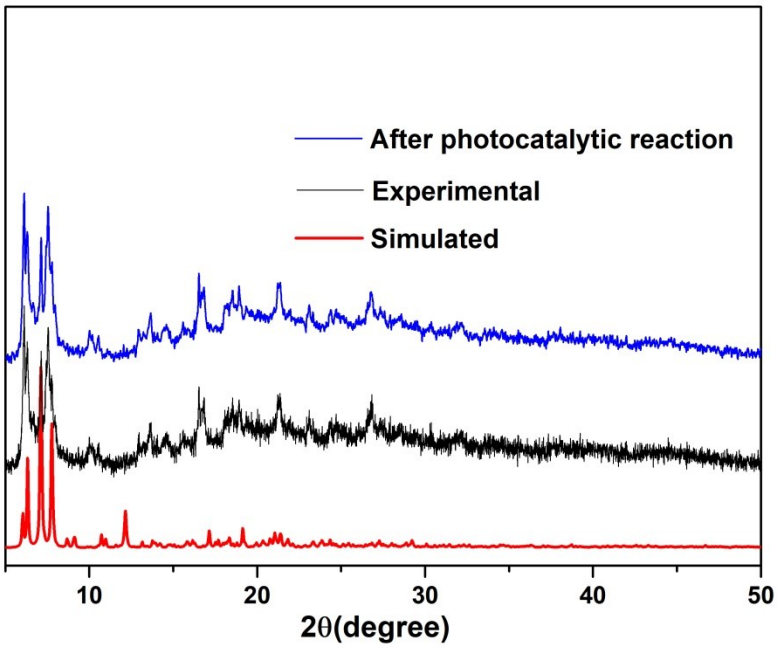

Figure S7 The XRD patterns of cluster **2** (the simulated pattern, as-synthesized product and sample **2** after photocatalytic experiment).

5. FT-IR spectrum

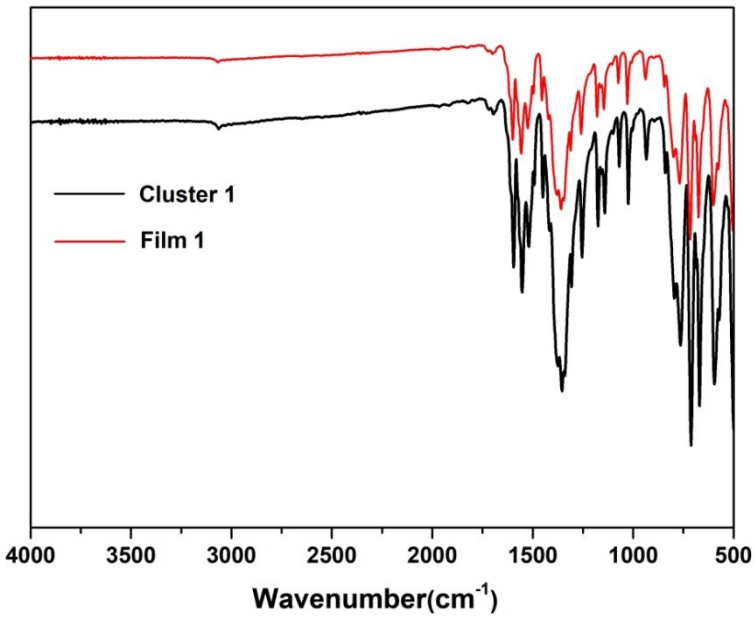

Figure S8 IR spectra of cluster **1** and the sample after photoelectrochemical experiment.

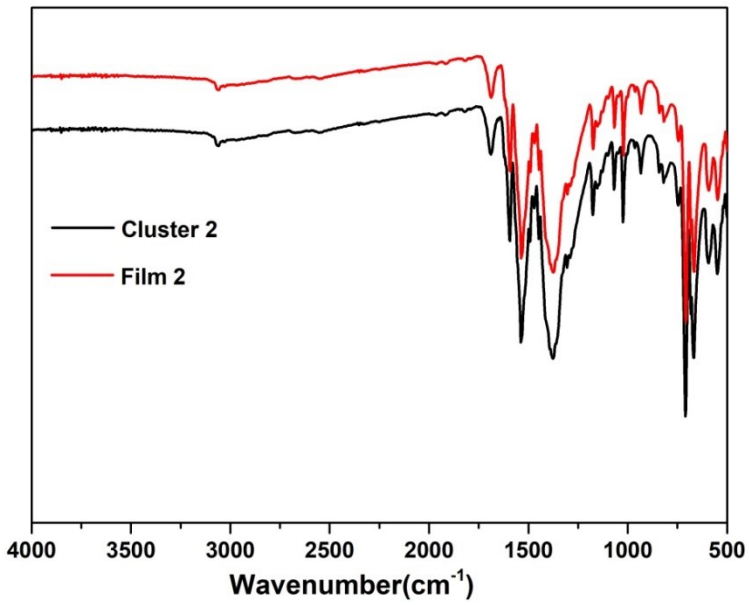

Figure S9 IR spectra of cluster **2** and the sample after photoelectrochemical experiment.

6. TG-Measurement

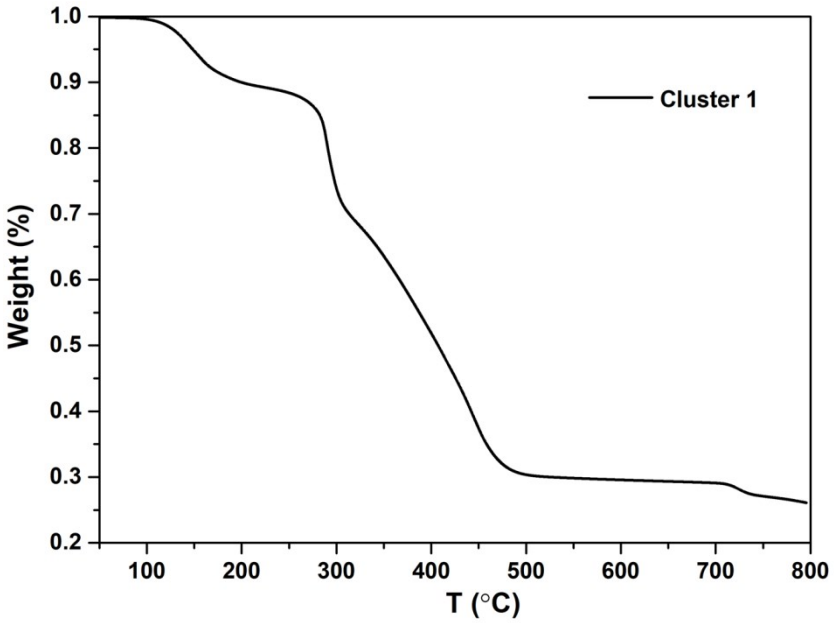

Figure S10 Thermal decomposition curve of cluster **1**.

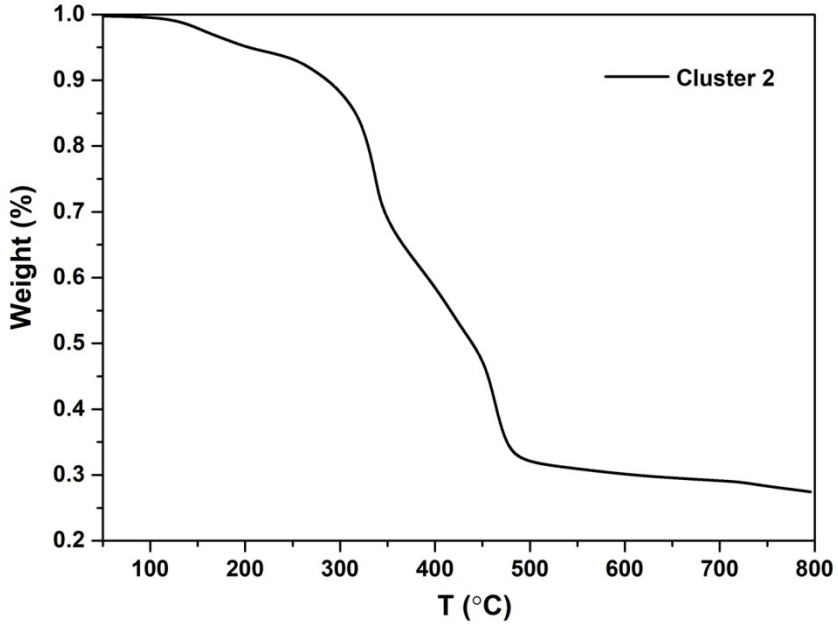

Figure S11 Thermal decomposition curve of cluster **2**.

7. DFT calculations

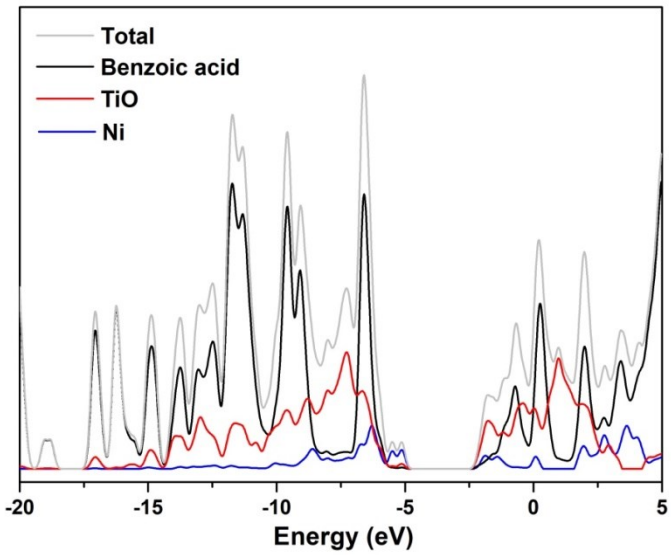

Figure S12 The density of state (DOS) plots for cluster **{Ti_8Ni_4+Ti_4Ni_2}**.

7. The incident photon-to-current conversion efficiency (IPCE)

The incident photon-to-current conversion efficiency (IPCE) was measured with the same three-electrode configuration. The electrodes **1** and **2** show the highest IPCE value of 0.12% and 0.08% (at 450 nm, Figure S). The IPCE of these clusters are lower than that of the related materials (J. Phys. Chem. C, 2014, 118, 25365; ACS Cent. Sci., 2020, 6, 1169), which can be attributed to their unique composition and structure.

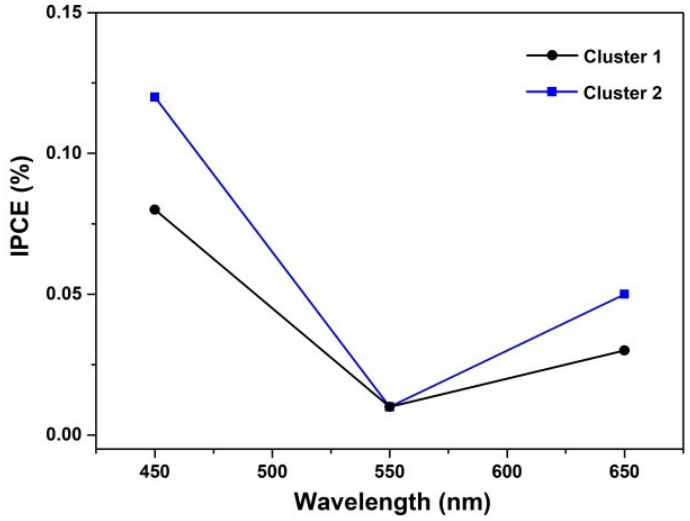

Figure S13 The IPCE values of clusters **1** and **2**.

8. Recycling H_2 evolution experiments

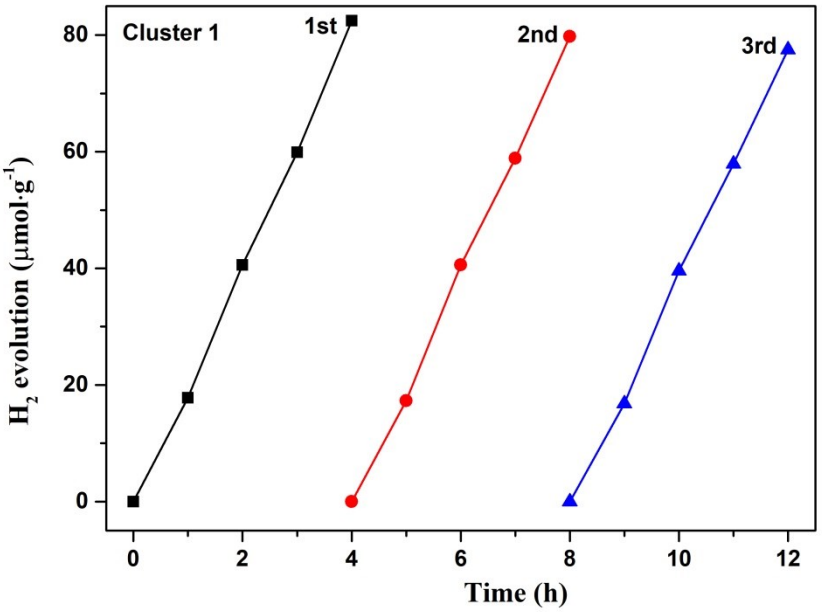

Figure S14 Recycling H_2 evolution experiments of cluster **1**.

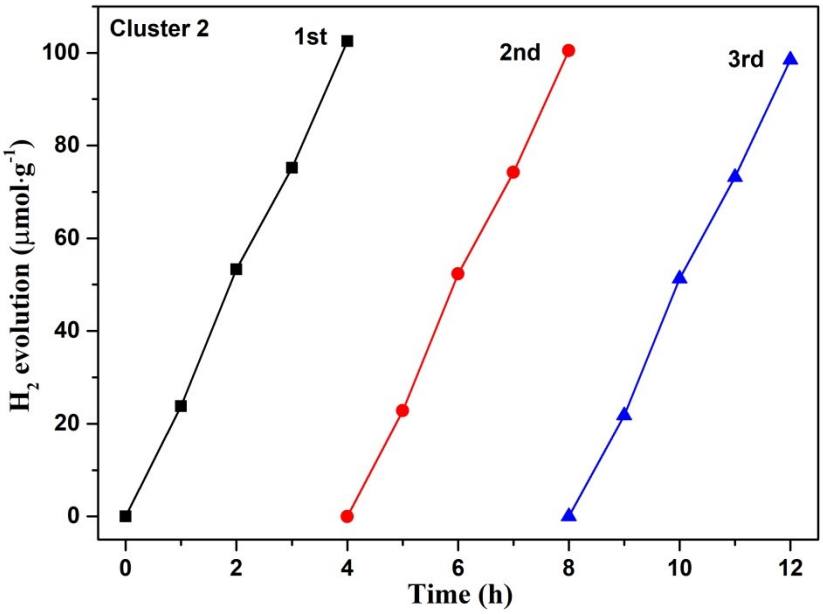

Figure S15 Recycling H_2 evolution experiments of cluster **2**.

9. Cartesian coordinates for {Ti_8Ni_4+Ti_4Ni_2}

The sub-cluster Ti_4Ni_2

Ni	-2.01032	0.35291	3.83116
Ti	0.282	-0.65363	2.24065
Ti	2.16613	-1.19888	-0.56628
O	1.25592	-0.47261	-2.05095
O	-0.63322	-2.20264	1.33859
O	1.21765	-0.30833	0.77537
O	1.12105	0.40275	3.55682
O	1.6912	-2.06435	2.75611
O	-1.08419	-1.28682	3.87692
O	4.1083	0.84879	-2.74406
O	0.68697	-2.65685	-0.45522
O	3.06782	-2.22492	0.95799
O	1.51266	-0.58575	5.5713
O	3.61504	-0.02932	-0.70809
O	2.67943	-2.12212	-3.91251
O	-2.70368	0.16235	5.5595
O	3.05135	-2.55761	-1.71452
C	-1.28887	-3.95719	-0.13763
C	2.80316	-2.43573	2.20549
C	1.65531	0.3842	4.79718
C	-0.35795	-2.87562	0.26005
C	2.42824	1.60217	5.16622
C	3.81205	-3.1276	3.0397
C	3.07888	-2.8936	-2.96674
C	-2.68487	-0.92306	6.26942
C	4.33727	0.76729	-1.51707
C	-2.02856	-2.11395	5.9005
H	-2.09803	-2.95849	6.57244
C	-1.23677	-2.256	4.76728
C	-2.49985	-4.13507	0.55465
H	-2.74271	-3.46358	1.36945
C	3.68148	-3.13334	4.44053
H	2.85357	-2.60319	4.89898
C	3.60281	-4.23342	-3.323
C	-0.95869	-4.8067	-1.20834
H	-0.02322	-4.65131	-1.73265
C	5.41587	1.53973	-0.84592
C	4.90902	-3.76179	2.42974
H	4.9989	-3.72943	1.35004
C	3.00796	1.67341	6.44517
H	2.86501	0.84281	7.12702
C	5.72403	-4.43034	4.61154
H	6.46552	-4.93713	5.22159
C	-0.49995	-3.5298	4.48515
H	-0.75704	-3.88958	3.48372
H	-0.73534	-4.29596	5.22621
H	0.57562	-3.33311	4.48366
C	3.91639	3.85551	5.91291
H	4.49432	4.72826	6.202
C	5.64269	1.41946	0.53543
H	5.02023	0.74803	1.11418
C	5.8586	-4.41638	3.2163
H	6.70258	-4.91088	2.74627
C	4.64014	-3.78446	5.22086
H	4.54579	-3.78201	6.3019
C	-3.37431	-5.15633	0.17627
H	-4.31656	-5.27925	0.69944
C	6.2152	2.40414	-1.61476
H	6.02942	2.47622	-2.6805
C	-3.42029	-0.83449	7.58272
H	-4.45918	-0.53962	7.39994
H	-2.96611	-0.05348	8.20302
H	-3.40144	-1.78013	8.12802
C	3.74883	2.79665	6.81631
H	4.19443	2.84914	7.8047

C	7.22921	3.14501	-1.00457
H	7.84817	3.80891	-1.59986
C	-3.03912	-6.00937	-0.88389
H	-3.71698	-6.80714	-1.17179
C	3.69074	-4.61881	-4.67194
H	3.37595	-3.91884	-5.4369
C	4.00532	-5.11938	-2.30874
H	3.9284	-4.80025	-1.27587
C	-1.83115	-5.83455	-1.57434
H	-1.57119	-6.49669	-2.39386
C	6.65959	2.16217	1.14197
H	6.83157	2.06909	2.20929
C	7.45198	3.02551	0.37471
H	8.2418	3.60095	0.84795
C	2.59336	2.6666	4.26406
H	2.13896	2.60412	3.28285
C	4.17899	-5.88468	-5.00141
H	4.24821	-6.18299	-6.04245
C	4.57954	-6.76828	-3.98978
H	4.95872	-7.75211	-4.24877
C	4.49226	-6.38455	-2.64486
H	4.80239	-7.07006	-1.86274
C	3.33821	3.78888	4.6389
H	3.46473	4.60595	3.93639
Ni	2.01032	-0.35291	-3.83116
Ti	-0.282	0.65363	-2.24065
Ti	-2.16613	1.19888	0.56628
O	-1.25592	0.47261	2.05095
O	0.63322	2.20264	-1.33859
O	-1.21765	0.30833	-0.77537
O	-1.12105	-0.40275	-3.55682
O	-1.6912	2.06435	-2.75611
O	1.08419	1.28682	-3.87692
O	-4.1083	-0.84879	2.74406
O	-0.68697	2.65685	0.45522
O	-3.06782	2.22492	-0.95799
O	-1.51266	0.58575	-5.5713
O	-3.61504	0.02932	0.70809
O	-2.67943	2.12212	3.91251
O	2.70368	-0.16235	-5.5595
O	-3.05135	2.55761	1.71452
C	1.28887	3.95719	0.13763
C	-2.80316	2.43573	-2.20549
C	-1.65531	-0.3842	-4.79718
C	0.35795	2.87562	-0.26005
C	-2.42824	-1.60217	-5.16622
C	-3.81205	3.1276	-3.0397
C	-3.07888	2.8936	2.96674
C	2.68487	0.92306	-6.26942
C	-4.33727	-0.76729	1.51707
C	2.02856	2.11395	-5.9005
H	2.09803	2.95849	-6.57244
C	1.23677	2.256	-4.76728
C	2.49985	4.13507	-0.55465
H	2.74271	3.46358	-1.36945
C	-3.68148	3.13334	-4.44053
H	-2.85357	2.60319	-4.89898
C	-3.60281	4.23342	3.323
C	0.95869	4.8067	1.20834
H	0.02322	4.65131	1.73265
C	-5.41587	-1.53973	0.84592
C	-4.90902	3.76179	-2.42974
H	-4.9989	3.72943	-1.35004
C	-3.00796	-1.67341	-6.44517
H	-2.86501	-0.84281	-7.12702
C	-5.72403	4.43034	-4.61154
H	-6.46552	4.93713	-5.22159
C	0.49995	3.5298	-4.48515
H	0.75704	3.88958	-3.48372

H	0.73534	4.29596	-5.22621
H	-0.57562	3.33311	-4.48366
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C	-5.64269	-1.41946	-0.53543
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C	-5.8586	4.41638	-3.2163
H	-6.70258	4.91088	-2.74627
C	-4.64014	3.78446	-5.22086
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C	3.37431	5.15633	-0.17627
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C	-6.2152	-2.40414	1.61476
H	-6.02942	-2.47622	2.6805
C	3.42029	0.83449	-7.58272
H	4.45918	0.53962	-7.39994
H	2.96611	0.05348	-8.20302
H	3.40144	1.78013	-8.12802
C	-3.74883	-2.79665	-6.81631
H	-4.19443	-2.84914	-7.8047
C	-7.22921	-3.14501	1.00457
H	-7.84817	-3.80891	1.59986
C	3.03912	6.00937	0.88389
H	3.71698	6.80714	1.17179
C	-3.69074	4.61881	4.67194
H	-3.37595	3.91884	5.4369
C	-4.00532	5.11938	2.30874
H	-3.9284	4.80025	1.27587
C	1.83115	5.83455	1.57434
H	1.57119	6.49669	2.39386
C	-6.65959	-2.16217	-1.14197
H	-6.83157	-2.06909	-2.20929
C	-7.45198	-3.02551	-0.37471
H	-8.2418	-3.60095	-0.84795
C	-2.59336	-2.6666	-4.26406
H	-2.13896	-2.60412	-3.28285
C	-4.17899	5.88468	5.00141
H	-4.24821	6.18299	6.04245
C	-4.57954	6.76828	3.98978
H	-4.95872	7.75211	4.24877
C	-4.49226	6.38455	2.64486
H	-4.80239	7.07006	1.86274
C	-3.33821	-3.78888	-4.6389
H	-3.46473	-4.60595	-3.93639

The sub-cluster Ti_8Ni_4

Ni	7.61028	2.51619	-0.03842
Ni	3.24397	-2.63137	0.99935
Ti	2.56541	0.0102	-0.55696
Ti	-0.16064	2.07577	-1.20053
Ti	6.05147	-0.42425	0.43029
Ti	5.21295	1.84619	-2.03948
O	6.23011	1.29843	-0.52732
O	4.33204	-0.48275	0.33265
O	2.82428	-1.4159	-1.92452
O	-1.79123	1.47564	-0.5234
O	3.67772	1.11477	-1.60157
O	-3.17851	2.08552	-2.8356
O	0.60693	2.66461	0.57322
O	0.94565	0.66024	-1.13381
O	2.39339	1.31184	0.96142
O	3.38515	-3.30698	-0.78652
O	-1.15465	3.96546	-1.14237
O	4.6608	-3.82627	1.47469
O	-0.93068	1.76914	-3.02151
O	6.31301	-2.28678	1.17535
O	6.39046	0.30009	2.16605
O	4.80488	3.60028	-1.15766

O	1.11736	3.2344	-2.20533
O	6.31533	-1.31637	-1.41334
O	5.96421	0.24701	-3.02259
O	4.79082	2.495	-3.87295
O	8.25784	-0.54668	0.30339
O	7.08115	2.83074	-2.58676
O	7.93353	1.93508	2.50299
O	9.0291	1.39969	-0.59199
O	6.36481	3.86258	0.47701
N	8.98939	3.79049	0.47169
C	5.89864	-3.46563	1.48996
C	1.58213	2.2519	1.32067
C	-2.30799	1.21895	-4.8846
C	-2.13883	1.71179	-3.49494
C	3.08746	-2.68586	-1.86995
C	6.34556	-0.93153	-2.63875
C	6.84944	-1.87537	-3.66851
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