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Electronic Supplementary Information for

Enhanced photocatalytic hydrogen production of microporous organic polymers by afterglow phosphorescent materials

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Experimental Section

General: SEM images were obtained using a JSM6700F microscope at the Chiral Material Core Facility Center of Sungkyunkwan University. PXRD patterns were obtained using a Rigaku MAX-2200 equipment. XPS spectra were obtained using a Thermo VG spectrometer. IR spectra were obtained using a Bruker VERTEX70 spectrometer. Solid ^{13}C NMR spectra (CP/TOSS) were obtained using a 500 MHz Bruker ADVANCE II NMR spectrometer. N_2 adsorption-desorption isotherm curves were obtained at 77K using a Micromeritics ASAP2020 equipment. The surface areas were characterized according to the BET theory. Pore size distribtuion diagrams were obtained by the NLDFT method. Reflectance spectra were obtained using a JASCO V-760 spectrometer. Emission spectra were obtained using a JASCO FP-6200 spectrometer. TGA analysis were conducted using a Seiko Exstar 7300 equipment. ICP-AES analysis was conducted using an OPTIMA8300 equipment. Emission decay curves were obtained at the KBSI (Daegu center) using a confocal MicroTime-200 microscope (Picoquant, Germany). A single-mode pulsed diode laser (375 nm with 30 ps pulse width, average power of 10 nW) was used as an excitation light source. A dichroic mirror (Z375RDC, AHF), a long pass filter (HQ405lp, AHF), a 75 μm pinhole, and an avalanche photodiode detector (PDM series, MPD) were used to collect emission photons. A time-correlated single-photon counting system (PicoHarp300, PicoQuant GmbH, Germany) was used to count the emission photons. Exponential fitting was conducted using the Symphotime-64 software (ver. 2.2). Steady-state PL spectrum was obtained by dividing and guiding emission photons through an optical fiber to the external spectrometer (F-7000, Hitachi). Photocurrents were measured using a CHI 660C equipment, a 300 W Xenon lamp as a light source, 0.1 M Na_2SO_4 as electrolyte, 5 wt% Nafion as a binder, FTO glass as a working electrode, Ag/AgCl as a reference electrode, and a Pt wire as a counter. EIS studies were conducted in the frequency range of 10^{-2}~10^5 Hz using a ZIVE sp1 equipment (WonAtech Co.).

Synthetic procedures of AG-MOP-TADS-Pds, MOP-TADS-Pd2, and AG-Pd

For the preparation of AG-MOP-TADS-Pd2, tris(4-trimethylstannylphenyl)amine and 3,7-dibromodibenzothiophene sulfone were prepared by the synthetic method reported in the literature.[1] AG (a commercial $Sr_4Al_{14}O_{25}$: Eu, Dy, B, PANAX Blue FB 800, UKSEUNG Chemical Co., 60 mg), $(PPh_3)_4Pd$ (37 mg, 32 μmol), and distilled DMF (20 mL) were added to a flame-dried 50 mL two-necked Schlenk flask under argon. After treating the reaction mixture with sonication for 30 min, tris(4-

trimethylstannylphenyl)amine (20 mg, 27 μmol) and 3,7-dibromodibenzothiophene sulfone (15 mg, 40 μmol) were added. The reaction mixture was stirred at 120 °C for 24 h. After being cooled to room temperature, the solid was separated by centrifugation, washed with a mixture of methylene chloride (10 mL) and methanol (30 mL) 8 times, and dried under vacuum.

For the preparation of AG-MOP-TADS-Pd1, the same synthetic procedures as AG-MOP-TADS-Pd2 were applied except using $(PPh_3)_4Pd$ (12 mg, 11 μmol). For the preparation of AG-MOP-TADS-Pd3, the same synthetic procedures as AG-MOP-TADS-Pd2 were applied except using $(PPh_3)_4Pd$ (74 mg, 64 μmol). For the preparation of MOP-TADS-Pd2, the same synthetic procedures as AG-MOP-TADS-Pd2 were applied without AG. For the preparation of AG-Pd, the same synthetic procedures as AG-MOP-TADS-Pd2 were applied without tris(4-trimethylstannylphenyl)amine and 3,7-dibromodibenzothiophene sulfone.

Experimental procedures of photocatalytic studies

Catalysts (3.00 mg of AG-MOP-TADS-Pd1, AG-MOP-TADS-Pd2, and AG-MOP-TADS-Pd3, 2.69 mg of AG, 2.88 mg of AG-Pd, 0.31 mg of MOP-TADS-Pd2, a mixture of 2.69 mg AG and 0.31 mg MOP-TADS-Pd2), triethanolamine (TEOA, 0.80 mL), distilled water (7.2 mL), and a spin bar were added to a tube-type glassware under nitrogen. The glassware was completely sealed with a rubber septum and a insulating tape. After treating with sonication for 30 min, the mixure was bubbled with N_2 gas for 15 min. The 1 mL of N_2 was replaced with 1 mL methane (an internal standard) using a GC syringe. The reaction mixutre was stirred at 21 ± 1 °C under irradiation of a 300W Xe lamp (Luxtel Ceralux CL300BF). The temperature of reaction mixture was carefully maintained at 25 °C with a water bath using the circulated water. After every 1 h, the amount of the generated hydrogen gas was analyzed using a GC (Agilent 6890) equipment with a thermal conductivity detector (TCD). The TCD detector has a different sensitivities towards hydrogen and methane. Thus, the detection sensitivity of the GC equipment was calibrated by the average value obtained using the same amount of hydrogen and methane. For the recycle tests of AG-MOP-TADS-Pd2, after the photocatalytic reaction for 5 h, the reaction mixture was bubbled with N_2 gas for 15 min to evacuate the generated hydrogen from the reaction mxiture. After sealing with a rubber septum, the 1 mL of N_2 was replaced with 1 mL methane (internal standard). Under irradiation, the gas was analyzed by GC (Agilent 6890). These procedures were repeated for the next run. The photocatalytic results were obtained through the statistical treatment of the five independent reactions. For the measurement of AQYs, a monochromatic light source was obtained using a band pass filter of 420 nm (420FS10-25). The AQYs were calculated based on the following equations.[2] AQY(%) = (number of reacted electrons × 100)/number of incident photons = (2×number of H_2 molecules×N_A×h×c×100)/(S×P×t×λ); N_A: Avogadro constant, h: Planck constant, c: speed of light, S: area value, P: light intensity, t: time, λ: wavelength. In our study, the light intensity at 420 nm was 5.86 mW/cm^2, respectively. The light intensities were measured by using a THORLABS PM100D. The irradiated area value was measured to be 7.73 cm^2.

Computational studies

To investigate the photocatalytic process of AG-MOP-TADS-Pds, the density functional theory (DFT) calculations were carried out. We designed the model systems (M-1~5) of MOP-TADS (Fig. 7a in the text)

M-1~4 correspond to the gradually extended molecular structures in which the triphenylamine (TA) and dibenzothiophene sulfone (DS) moieties are alternatively connected with π-conjugation. On the other hand, M-5 represents a branched networking case. We tried to determine the ionization potentials of ground state (IP) and ionization potentials of excited state (IP*) for the MOP-TADS. Especially IP* value is the most significant factor which determines the possibility of photocatalytic proton reduction reaction. Firstly, the neutral and cationic ground states for M-1~5 model systems were optimized at the B3LYP/6-31G* level. Then, the time-dependent density functional theory (TD-DFT) calculations were conducted to obtain the solution of the 1st excited state. The Tamm-Dancoff approximation (TDA) was used to reduce the instability of excited states in the calculations. For all DFT calculations regarding M-1~5, the Gaussian 16 program package was used.[3] The IP and IP* were computed based on the following equation:

$$IP = E(M^+) - E(M),\ IP^* = E(M^+) - E(M^*) \quad (1)$$

Herein E(M), E(M^+) and E(M*) denote the self-consistent field (SCF) energies of fully optimized neutral ground state, cationic ground state, and the 1st excited state of M-1~5, respectively. Then, the calculated potential energies ($Ø_{vac}$) relative to the vacuum level were converted to those values ($Ø_{NHE}$) relative to the normal hydrogen electrode (NHE) potential by using the following equation.[4]

$$\phi_{NHE} = -4.85 - \phi_{vac} \quad (2)$$

The calculated IP and IP* energy levels of M-1~5 were located at around 0.64 ~ 0.79 eV and -1.65 ~ -1.89 eV, respectively (Fig. 7b in text). We found that IP and IP* were gradually converged to certain values for M-3~5 with increase in π-conjugation length. Thus, the representative values of IP and IP* of MOP-TADS can be the average values for M-3~5, that is 0.68 eV and -1.87 eV, respectively. Consequently, the IP and IP* on NHE potential scale were depicted in Fig. 7d in text.

To estimate the energy levels of electronic structure for afterglow (AG) materials on the scale of NHE potential, the bulk unit cell and surface slab model for $Sr_4Al_{14}O_{25}$ having *Pmma* space group[5] were optimized at PBE/light tier-1 level of theory within a periodic boundary condition (PBC) using the FHI-aims code.[6] The 3×3×3 Monkhorst-Pack *k*-points meshes and the convergence criteria 0.02 eV/Å were used. With consideration of heavy metal atoms, the relativistic effects were treated at the zeroth order regular approximation (ZORA) level scale.[7] For the bulk unit cell, the geometrical optimizations of both nucleus positions and lattice parameters were conducted. The fully optimized lattice parameters of bulk unit cell for $Sr_4Al_{14}O_{25}$ are a = 24.764 Å, b =8.514 Å, c = 4.901 Å and $\alpha = \beta = \gamma$ = 90.000 ° (Fig. S10). The surface slab model of $Sr_4Al_{14}O_{25}$ was designed with 1×2×2 duplication of the optimized unit cell by cutting the facet with (010) plane. Then, along the z-axis a vacuum space of 20 Å was added to avoid spurious interaction between slab models in PBC. We also considered the slab models of (100) and (001) surfaces of $Sr_4Al_{14}O_{25}$ possessing same number of atoms in the designed (010) surface. However, it was found that the slab model of (100) surface has much higher SCF energy than (010) surface by 50.05 eV, that indicates thermodynamic instability of (100) surface. And the geometrical optimization process of the slab model of (001) surface gets the severe convergence problem. Hence, it is notable that the DFT results of the slab models of (100) and (001) surfaces were omitted in this study.

To align the ionization potential of AG materials relative to NHE potential, firstly we determined the valence band maximum (VBM) level of bulk $Sr_4Al_{14}O_{25}$. However, normally the vacuum reference level cannot be defined in PBC calculations especially for a bulk unit cell. To solve this problem, we added a He atom as a reference atom above the optimized (010) surface slab model with distance of 10 Å inducing no atomic interaction. Then, a single point calculation was carried out to obtain the density of state (DOS) at PBE/light-tier1 level relative to the energy level of 1s orbital of a He atom in vacuum level (-15.76 eV), as shown in Fig. S11 in the ESI. It should be noted that we tried to assign the VBM level of bulk $Sr_4Al_{14}O_{25}$ instead of that of (010) surface. Thus, the DOS of bulk unit cell was aligned to the DOS of (010) surface in vacuum level with consideration of matching the maximum peak near to VBM remarked as $Peak_{max}$ in Fig. S11 in the ESI. The partial density of state (pDOS) plots shows that the valence bands of bulk unit cell and (010) surface slab model are dominantly composed of O p-orbital state (Fig. S12 in the ESI). In other words, we used the $Peak_{max}$ positions of DOS consisting of O p-orbital states in valence bands to match the bulk DOS and surface DOS. Finally, we defined the position of VBM of bulk unit cell as -5.59 eV relative to a vacuum level.

Based on the Koopman's theorem, the negative VBM value of solid is approximately considered as the IP value relative to a vacuum level. Then, using equation (2) the estimated IP is adjusted to the scale of NHE potential shown as 0.74 eV in Fig. 7d in text. The position of excited state of $Sr_4Al_{14}O_{25}$ was estimated from the band gap value of bulk $Sr_4Al_{14}O_{25}$. To estimate more reliable band gap value of bulk $Sr_4Al_{14}O_{25}$, a single point calculation with B3LYP/light tier-1 level and 3×3×3 *k*-point mesh was performed based on the optimized structure at PBE/light-tier1 level. (Calc. 5.96 eV in Fig. 7d in text) According to previous theoretical study, it is known that the green luminescent of AG materials is originated in the doped Eu^{2+} states.[8] Considering the experimentally observed energy range of photo-luminescent (PL), that is Expt. 2.08 eV ~ 3.09 eV, we finalized the schematic figure of photocatalytic mechanism including the optical transition from doped Eu^{2+} states in $Sr_4Al_{14}O_{25}$, as shown in Fig. 7d in text.

Reference

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Fig. S1 (a) Pd and (b) AG amount dependent photocatalytic performance of MOP-TADS-Pd.

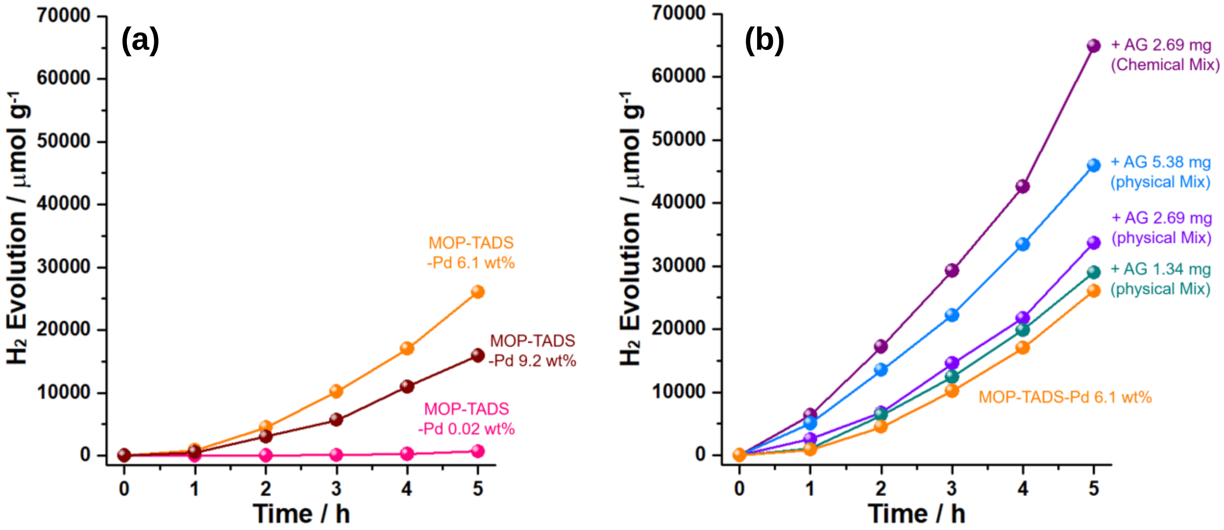


Fig. S2 Characterization data of AG-Pd: (a) PXRD pattern and XPS spectrum of AG-Pd.

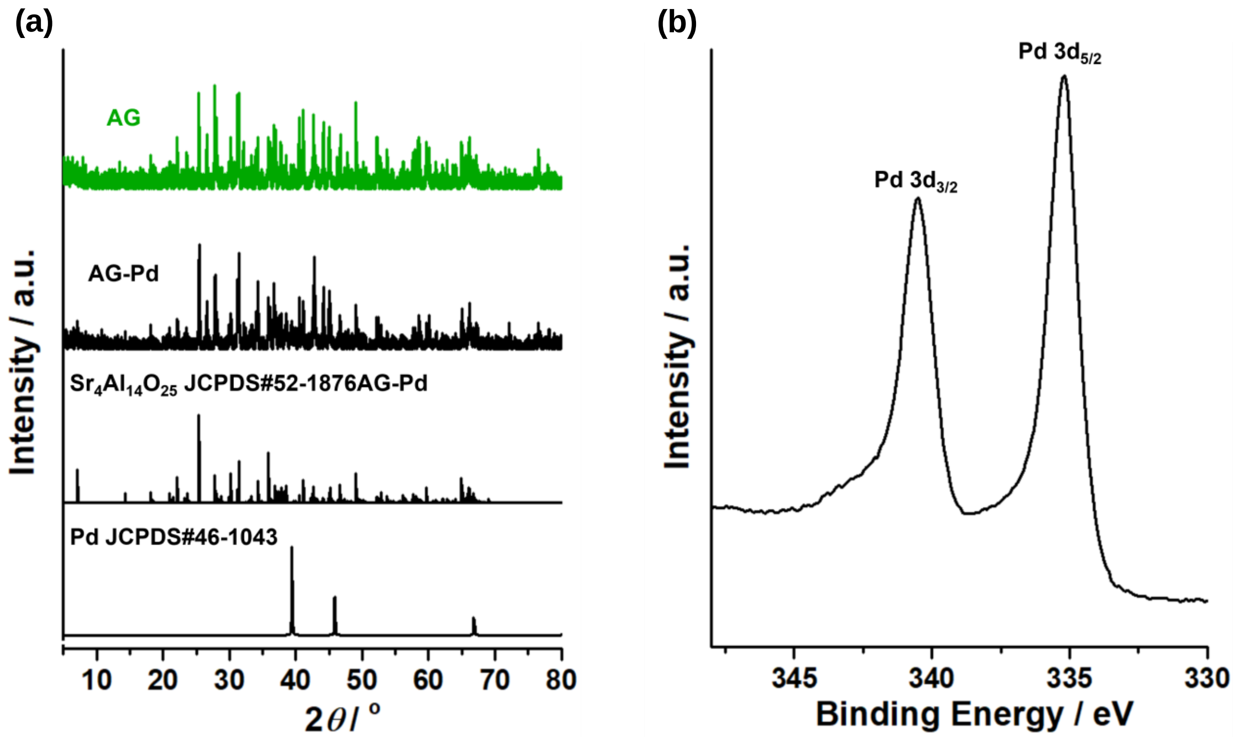


Fig. S3 TEM and HR-TEM images of Pd nanoparticles on MOP-TADS.

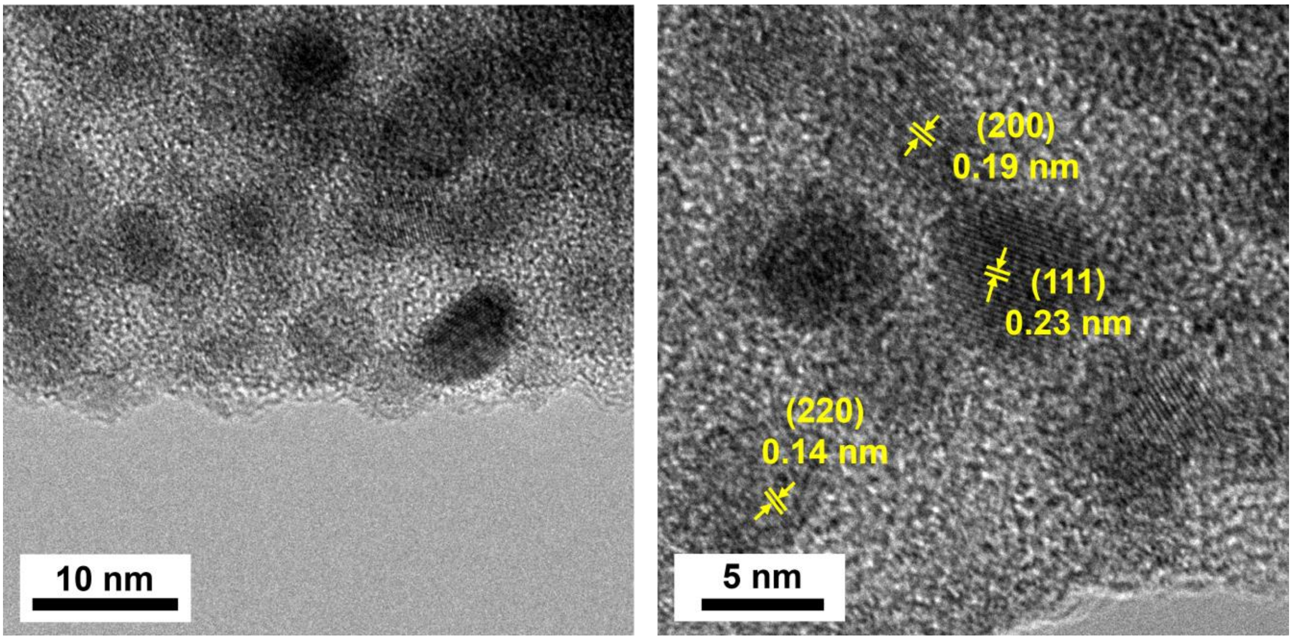


Fig. S4 The PXRD pattern of MOP-TADS obtained through Pd etching from MOP-TADS-Pd2.

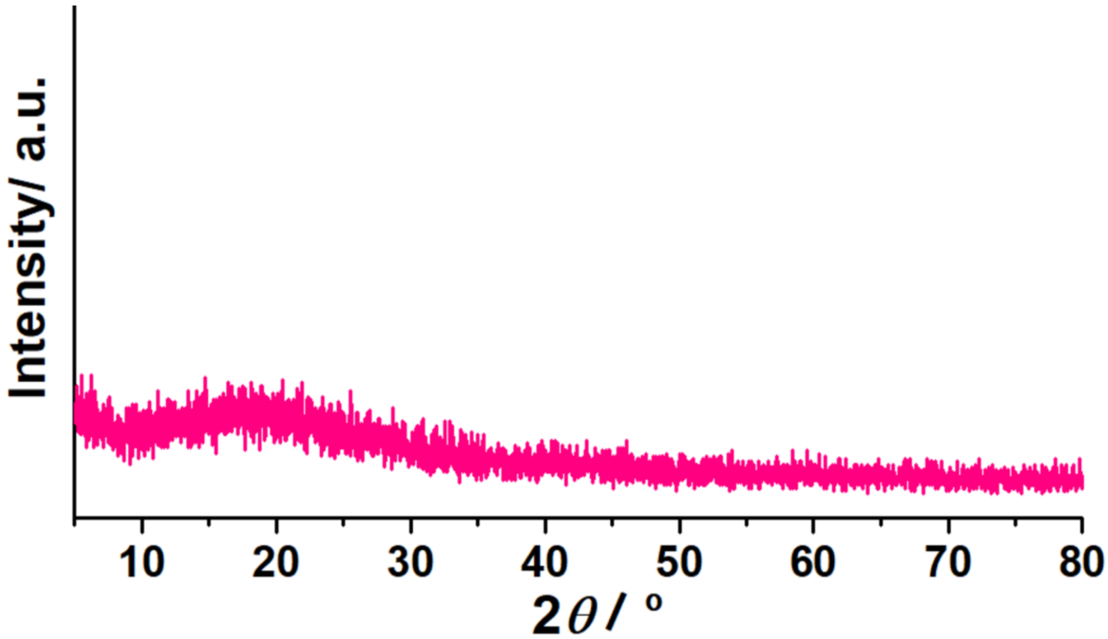


Fig. S5 XPS survey spectra of AG-MOP-TADS-Pds, MOP-TADS-Pd, and AG.

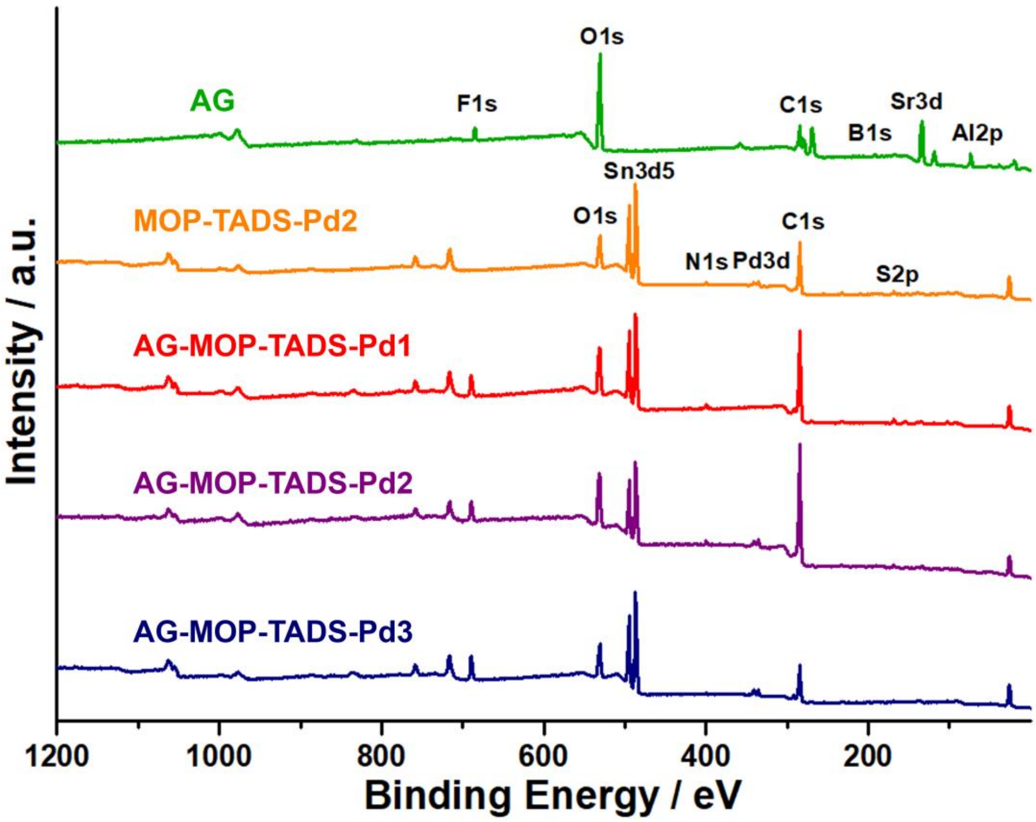


Fig. S6 N_2 adsorption-desorption isotherm curves of MOP-TADS obtained through Pd etching from MOP-TADS-Pd2.

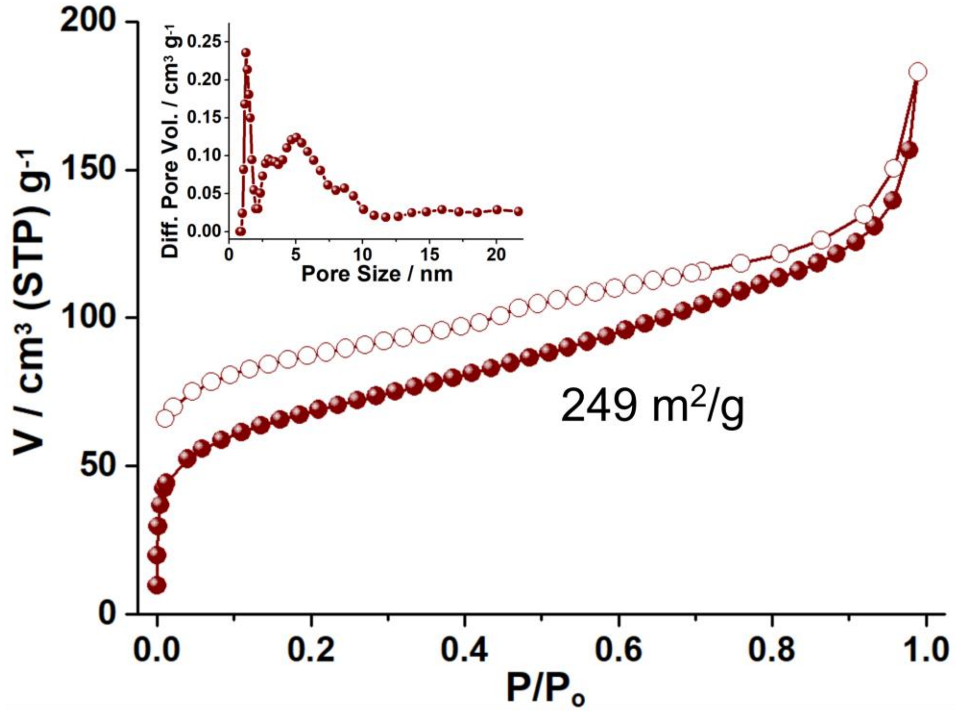
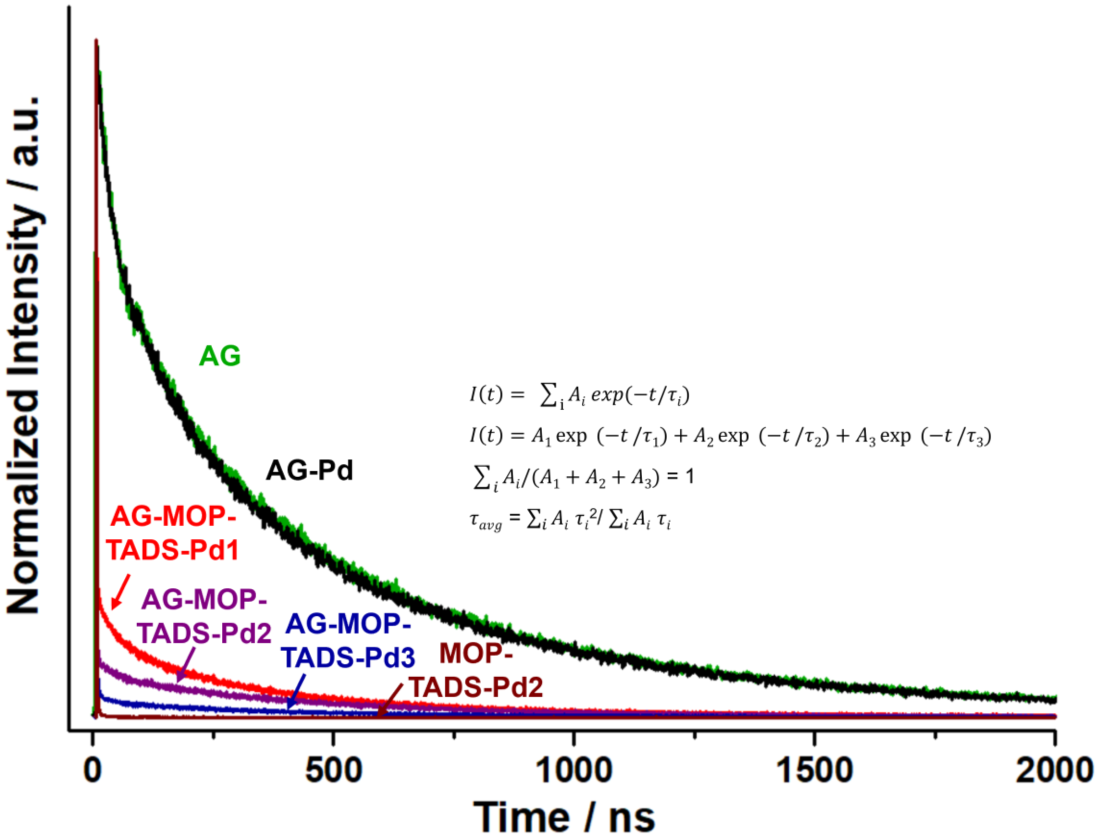


Fig. S7 The analysis of emission lifetime of AG, AG-MOP-TADS-Pds, MOP-TADS-Pd2, and AG-Pd.



	τ_1 (ns)	A_1 (%)	τ_2 (ns)	A_2 (%)	τ_3 (ns)	A_3 (%)	τ_{avg} (ns)
AG	752	33	268	38	30	29	360
AG-Pd	727	36	242	37	35	27	362
AG-MOP-TADS-Pd1	383	8.3	60	6.7	0.40	85	36
AG-MOP-TADS-Pd2	446	4.9	33	2.5	0.37	93	23
AG-MOP-TADS-Pd3	387	2.0	9.4	3.4	0.41	95	8.5
MOP-TADS-Pd2	37	0.16	3.1	6.2	0.39	94	0.62

Fig. S8 (a) IR and (b) XPS spectra of AG-MOP-TADS-Pd2 before and after 5 recycle tests.

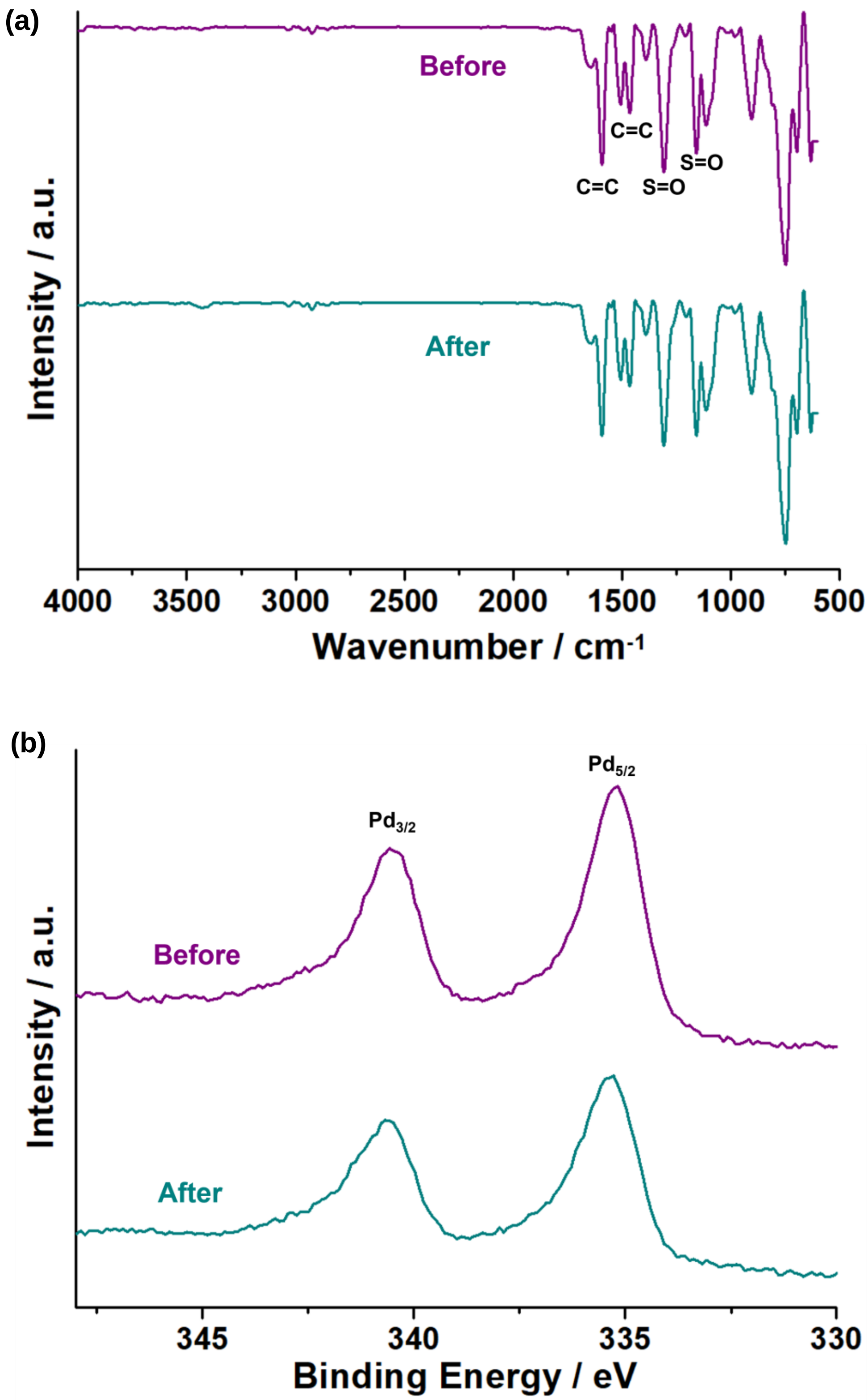


Fig. S9 The optimized structures of bulk (up) and (010) surface slab model (down) of $Sr_4Al_{14}O_{25}$.

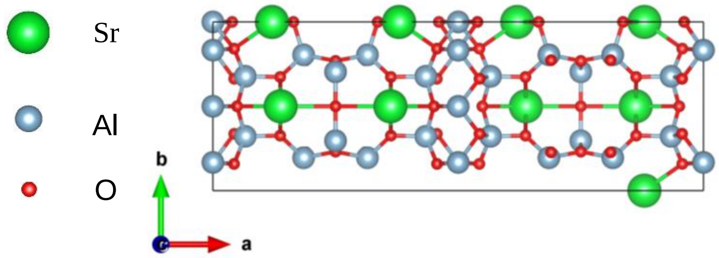
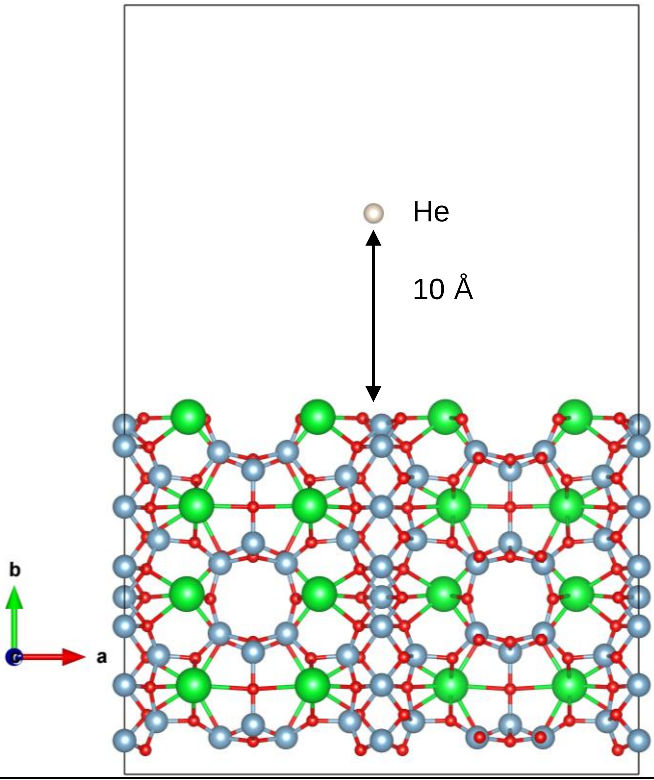
Bulk $Sr_4Al_{14}O_{25}$	
Slab model of (010) surface for $Sr_4Al_{14}O_{25}$	

Fig. S10 The valance band maximum (VBM) level of bulk $Sr_4Al_{14}O_{25}$ estimated from the density of state (DOS) plots calculated at PBE/light-tier1 level in comparison of DOS plot of (010) surface slab model of $Sr_4Al_{14}O_{25}$.

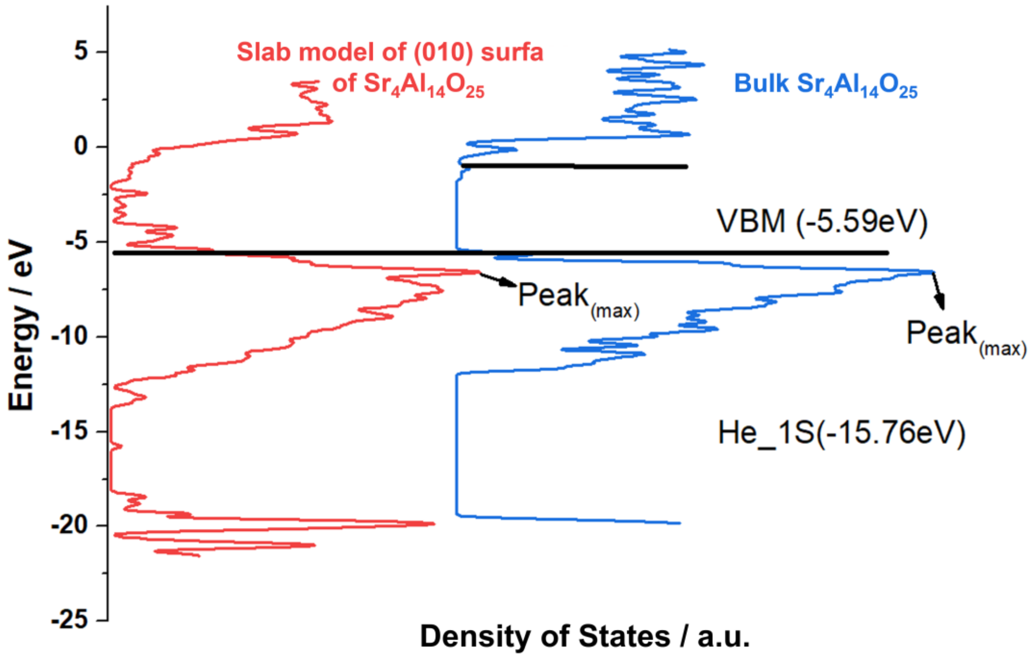


Fig. S11 The calculated atom-projected and angular-momentum resolved partial density of state (p-DOS) plots for the bulk (a and b) and (010) surface slab (c and d) for $Sr_4Al_{14}O_{25}$.

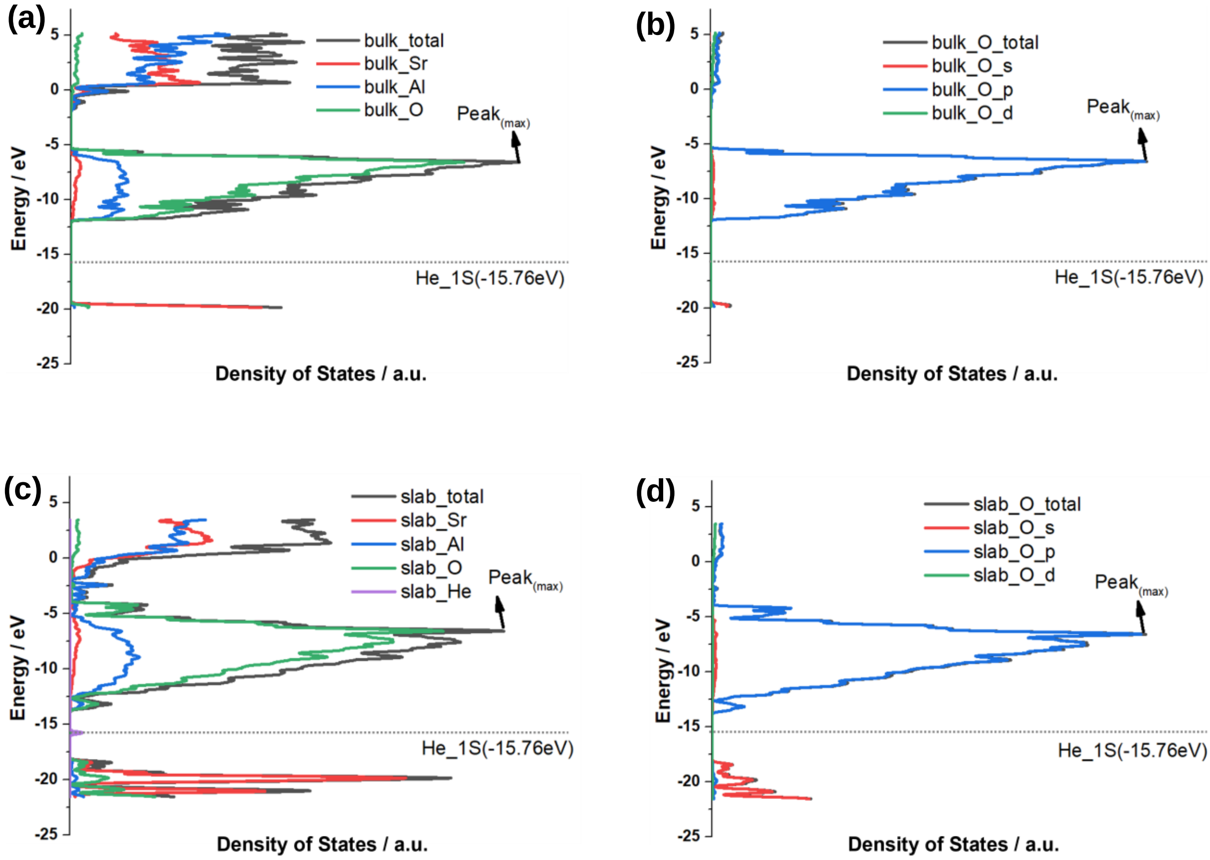


Fig. S12 Cartesian coordinates (in Å) of optimized model systems (TA, DS, M-1~5 and $Sr_4Al_{14}O_{25}$).

TA

N 0.00005900 -0.00005400 -0.00172700
C 0.34575300 -1.37901500 -0.00064700
C -0.35909000 -2.29199400 -0.80208500
C 1.39764800 -1.85069100 0.80164200
C -0.02237100 -3.64416200 -0.79093400
H -1.16887000 -1.93500300 -1.43042900
C 1.73891500 -3.20174900 0.79164300
H 1.94301800 -1.15332400 1.42953500
C 1.03025500 -4.10855000 0.00062800
H -0.57930200 -4.33570100 -1.41794400
H 2.55605700 -3.54814400 1.41921300
H 1.29453600 -5.16218700 0.00108000
C -1.36705100 0.39004300 -0.00068900
C -2.30061300 -0.28244400 0.80479800
C -1.80609500 1.45408900 -0.80544700
C -3.64130800 0.09755600 0.79498900
H -1.96848700 -1.10140100 1.43488200
C -3.14544900 1.83866500 -0.79421100
H -1.09259500 1.97456600 -1.43635600
C -4.07301400 1.16202600 0.00077200
H -4.34926600 -0.43478000 1.42502900
H -3.46661800 2.66457400 -1.42370000
H -5.11761500 1.46003600 0.00134600
C 1.02130100 0.98904700 -0.00089900
C 0.90440600 2.13487800 0.80284200
C 2.16347200 0.83629700 -0.80382700
C 1.90392200 3.10585600 0.79340300
H 0.02831600 2.25764700 1.43163800
C 3.16629900 1.80383800 -0.79211300
H 2.25840800 -0.04273600 -1.43336400
C 3.04295000 2.94642500 0.00130000
H 1.79594200 3.98594600 1.42215000
H 4.04306500 1.66819100 -1.42013900
H 3.82341500 3.70198900 0.00215700

DS

C 2.98551700 -1.83299200 -0.00015000
C 3.51150700 -0.53732100 -0.00015200
C 2.65704200 0.57005400 -0.00010200
C 1.29114400 0.33414700 -0.00005500
C 0.73941600 -0.95460900 -0.00004900
C 1.60532100 -2.05060200 -0.00009800
H 3.65918800 -2.68520000 -0.00019000
H 4.58717400 -0.38855800 -0.00018900
H 3.04874900 1.58258500 -0.00010100
H 1.21469900 -3.06409100 -0.00009100
C -1.29114400 0.33414800 0.00006700
C -2.65704200 0.57005500 0.00012600
C -3.51150700 -0.53732000 0.00014100
C -2.98551800 -1.83299100 0.00009100
C -1.60532100 -2.05060200 0.00002900
C -0.73941600 -0.95460800 0.00001600
H -3.04874900 1.58258600 0.00016000
H -4.58717400 -0.38855600 0.00019100
H -3.65918900 -2.68519900 0.00009900
H -1.21470000 -3.06409100 -0.00001100
S 0.00000000 1.58883500 0.00002400
O 0.00006800 2.33404500 1.26810700
O -0.00006700 2.33408100 -1.26803700

M-1

C 2.99096000 0.00451500 2.05364500
C 3.54092300 0.00837400 0.75632600
C 2.65275900 0.00812200 -0.33819700
C 1.29174500 0.00809000 -0.09734900
C 0.73683300 0.00168600 1.19055500
C 1.61495200 -0.00143600 2.27730700
H 3.66085600 0.03167900 2.90782500
H 3.03107300 -0.01754500 -1.35523700
H 1.23504800 0.00277300 3.29512700
C -1.29174400 -0.00810200 -0.09734900
C -2.65275800 -0.00813900 -0.33819600
C -3.54092200 -0.00836800 0.75632700
C -2.99095800 -0.00448300 2.05364600
C -1.61495000 0.00147300 2.27730700
C -0.73683100 -0.00167200 1.19055500
H -3.03107200 0.01750900 -1.35523700
H -3.66085400 -0.03162800 2.90782700
H -1.23504600 -0.00271600 3.29512700
S 0.00000000 -0.00002000 -1.35263400
O -0.00628900 1.26758200 -2.09937100
O 0.00628900 -1.26763900 -2.09934200
C -5.00608300 -0.01300500 0.54302200
C -5.58488100 -0.71341600 -0.52982900
C -5.87399000 0.68349400 1.40191600
C -6.95824700 -0.71450900 -0.74166400
H -4.95125800 -1.28015200 -1.20641000
C -7.24987300 0.67875200 1.20658400
H -5.46557900 1.25452300 2.23116400
C -7.81810000 -0.01894700 0.12630300
H -7.37328300 -1.26207600 -1.58128200
H -7.89318300 1.22546900 1.88803700
N -9.21760500 -0.02051100 -0.08178300
C -9.87019100 -1.19282000 -0.55984000
C -9.98420200 1.15142900 0.17658100
C -9.55608800 -2.45195400 -0.02448900
C -10.84226300 -1.10310100 -1.56829000
C -11.21764700 1.06027200 0.84037100
C -9.52270600 2.41168100 -0.23548100
C -10.19464700 -3.59603000 -0.49945200
H -8.81169300 -2.52656700 0.76198700
C -11.48901700 -2.25057200 -2.02378900
H -11.08524900 -0.13267500 -1.98937100
C -11.97351400 2.20676400 1.07819200
H -11.57730200 0.08902600 1.16502000
C -10.27685400 3.55467500 0.02339900
H -8.57445100 2.48827100 -0.75807800
C -11.16711500 -3.50336600 -1.49748700
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M-2

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M-3

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M-4

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C -18.82046600 2.71068700 1.20088900
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H -19.38874100 2.68872700 2.12649200
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H -19.66222300 4.97072900 3.02714400
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H -16.62154400 5.23443300 -1.94651300
H -15.61110100 5.98561100 2.16606700
N -17.63650000 6.01593300 0.40931400
C -18.70624100 5.33520400 -0.23935000
C -17.93279500 7.05714200 1.33579800
C -18.69399700 3.93673600 -0.36098900
C -19.79350400 6.05612300 -0.75706700
C -18.94758900 6.88908600 2.29047500
C -17.22088300 8.26635100 1.30108300
C -19.74381500 3.27870300 -0.99917900
H -17.86121700 3.37286600 0.04739800
C -20.84757100 5.38778400 -1.37720800
H -19.80594000 7.13781400 -0.66822300
C -19.24506400 7.91457400 3.18622500
H -19.49807600 5.95417700 2.32430200
C -17.51286900 9.27924200 2.21276200
H -16.44120100 8.40516600 0.55866100
C -20.82807200 3.99752000 -1.50724600
H -19.71930400 2.19550700 -1.08466600
H -21.68227400 5.96077700 -1.77243200
C -18.52804200 9.11255700 3.15724500
H -20.03354400 7.76860900 3.91983700
H -16.95189200 10.20927200 2.17332000
H -21.64817100 3.48040900 -1.99709400
H -18.75778900 9.90675600 3.86176900

$Sr_4Al_{14}O_{25}$

Sr 2.98149215 -0.00031133 4.35489083
Sr 21.78272148 0.00112208 0.54978714
Sr 9.40022051 0.00007723 4.35575623
Sr 15.36420667 0.00056864 0.54874541
Sr 3.41940301 4.25702037 4.70827114
Sr 21.34425741 4.25830766 0.19646579
Sr 8.96155513 4.25721539 4.70902823
Sr 15.80216946 4.25779171 0.19559694
Al 1.63346855 2.74252550 2.41497155
Al 23.13029642 5.77266391 2.48988514
Al 10.74827833 5.77172597 2.41619524
Al 14.01546258 2.74314548 2.48828919
Al 23.13037851 2.74388800 2.48959077
Al 1.63306187 5.77141886 2.41479119
Al 14.01525753 5.77200771 2.48839830
Al 10.74848337 2.74292131 2.41619871
Al 4.57938610 1.65840282 1.83351077
Al 20.18430355 6.85666421 3.07139658
Al 7.80246210 6.85574125 1.83389540
Al 16.96125460 1.65909333 3.07063265
Al 20.18462040 1.65932224 3.07111736
Al 4.57900996 6.85563307 1.83345653
Al 16.96086913 6.85642300 3.07087268
Al 7.80277725 1.65847891 1.83397922
Al 0.00030943 1.42426919 0.00005416
Al -0.00020548 7.08945161 0.00014603
Al 12.38208059 7.08995105 0.00196441
Al 12.38245437 1.42478057 0.00187791
Al 6.19063559 2.51723830 4.27230487
Al 18.57300879 5.99786304 0.63261473
Al 6.19042568 5.99691355 4.27220636
Al 18.57327621 2.51816301 0.63237492
Al 0.00014138 -0.00027297 2.45048397
Al 12.38228661 0.00037019 2.45243876
Al 0.00023489 4.25647066 -0.00025277
Al 12.38224163 4.25737369 0.00178684
O 1.07760812 2.86888475 0.73074202
O 23.68626114 5.64662728 4.17426560
O 11.30468527 5.64552895 0.73208359
O 13.45900975 2.86909354 4.17247295
O 23.68611690 2.87003776 4.17396693
O 1.07701422 5.64537885 0.73050744
O 13.45883087 5.64569433 4.17251410
O 11.30483948 2.86902283 0.73204778
O 1.06791613 1.34781234 3.32180746
O 23.69563228 7.16756402 1.58312848
O 11.31348498 7.16649595 3.32316611
O 13.45028737 1.34830964 1.58130038
O 23.69626407 1.34916521 1.58294332
O 1.06751413 7.16615540 3.32166203
O 13.44992755 7.16674265 1.58139375
O 11.31400690 1.34818621 3.32305726
O 3.39601620 2.77737953 2.46343297
O 21.36767485 5.73755099 2.44164793
O 8.98566785 5.73662934 2.46393132
O 15.77803734 2.77801963 2.44033599
O 21.36781607 2.77838049 2.44101047
O 3.39565548 5.73649308 2.46313314
O 15.77787049 5.73717178 2.44068795
O 8.98590613 2.77747261 2.46430571
O 4.68918512 1.93471695 0.09107593
O 20.07439305 6.58045371 4.81383387
O 7.69311072 6.57963192 0.09139217
O 17.07063570 1.93547618 4.81305559
O 20.07472128 1.93575321 4.81347172
O 4.68893417 6.57950707 0.09097807
O 17.07028652 6.58021251 4.81334033
O 7.69334523 1.93486863 0.09155233
O 0.97411009 -0.00022479 0.83848928
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O 11.40867657 -0.00002945 0.83995951
O 13.35574357 0.00005794 4.06454880
O 1.22128390 4.25690697 3.31460537
O 23.54229631 4.25829013 1.59008082
O 11.16010952 4.25732267 3.31601108
O 13.60370381 4.25752318 1.58849519
O 4.06281768 -0.00023259 2.06948799
O 20.70165494 0.00081788 2.83532115
O 8.31953844 -0.00007165 2.07006671
O 16.44454596 0.00051317 2.83464572
O 6.19097120 1.96753416 2.56553292
O 18.57272896 6.54763815 2.33935750
O 6.19064497 6.54649509 2.56538091
O 18.57302561 1.96806626 2.33901830
O 6.19051909 4.25707894 4.37980231
O 18.57315349 4.25802307 0.52517512

Table S1. HER and AQYs of the reported MOP-based photocatalysts (Referring to the recent review paper[1] of CMP-based photocatalysts for hydrogen evolution).

MOP-based Photocatalysts	Metal Catalyst	Light Source	HER (μmol h^{-1} g^{-1})	AQY(@420 nm) (%)	Year	Ref
VH-MON **(Our work)**	Pt	200 W Xe	1250		2014	2
CP-CMP10	Pd	300 W Xe	174	0.42	2015	3
B-BT-1,3,5	Pd/Pt	300 W Xe	400		2016	4
PCP4e	Pd	150 W Xe	1900	0.34 (@350 nm)	2016	5
PCP2-100%PDI	Pd/Cu	150 W Xe	2171		2016	6
PCP2-100%PDI	Pd/Cu	150 W Xe	3142		2016	7
SP-CMP	Pd	300 W Xe	120	0.23	2016	7
PTEB	Cu	300 W Xe	102		2017	8
PTEPB	Cu	300 W Xe	218		2017	9
PrCMP-3	Pt	300 W Xe	121		2017	9
PrPy	Pt	300 W Xe	3020		2017	10
aza-CMP/C2N	N/A	300 W Xe	100	4.3 (@600 nm)	2018	11
PyDOBT-1	Pd	300 W Xe	5697		2018	12
PyDOBT-1	Pt	300 W Xe	8523		2018	13
DBTD-CMP1	Pd	300 W Xe	2460		2018	13
DBTD-CMP1	Pt	300 W Xe	4600		2018	14
S-CMP3	Pd	300 W Xe	3106	13.2	2019	14
BDP-bdy-TPA	Pd	300 W Xe	2780		2020	15
H-MOP@SCMP-Pd2 **(Our work)**	Pd	300 W Xe	7100	3.72	2021	16
BTT-CPP	Pd	300 W Xe	12633	3.3 (@365 nm)	2021	17
PyBS-3	Pd	300 W Xe	430		2021	18
Py-TPA-CMP	Pt	350 W Xe	19200	15.3	2021	19
PyDTDO-3	Pt	300 W Xe	16320	3.7	2021	20
TPE-SOBT	Pd	300 W Xe	2990	3.88	2021	21
30%@Co@PCMP	Co	300 W Xe	17200	2.05	2021	22
DBC-BTDO	Pd	300 W Xe	49340	26.58 (@450 nm)	2022	23
BSO_2-EDOT	Pd	300 W Xe	158400	13.6 (@550 nm)	2022	24
BTPT-CMP1	Pt	300 W Xe	5561	3.8	2022	25
Py-T-BTDO-3	Pt	300 W Xe	78400	29.79	2022	26
PySO-2	Pd	300 W Xe	23300	17.7	2022	27
PF6A-SF	Pd	300 W Xe	17460	1.26	2022	28
MOP-TADS-Pd2 **(Our work)**	Pd	300 W Xe	5270		2022	This work
AG-MOP-TADS-Pd2 **(Our Work)**	Pd	300 W Xe	12900[a]	1.02	2022	This work

a HER value based on the MOP-TADS-Pd2.

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