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Electronic Supplementary Information (ESI)

Molecular layer deposition of photoactive metal-naphthalene hybrid thin films

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1. X-ray reflectivity (XRR)

The XRR fitting process was performed using X'Pert Reflectivity software. The sample model used for fitting consisted of three layers: Si substrate, SiO_2 native oxide layer and deposited film layer. Each new system i.e. Ti-, Y-, Zr-, and Hf-NDC was created and added to the material database. The fitted parameters for each layer were thickness, density and roughness. The instrument parameters such as substrate length (10 mm) and beam width (0.1 mm) were also added to the fitting process.

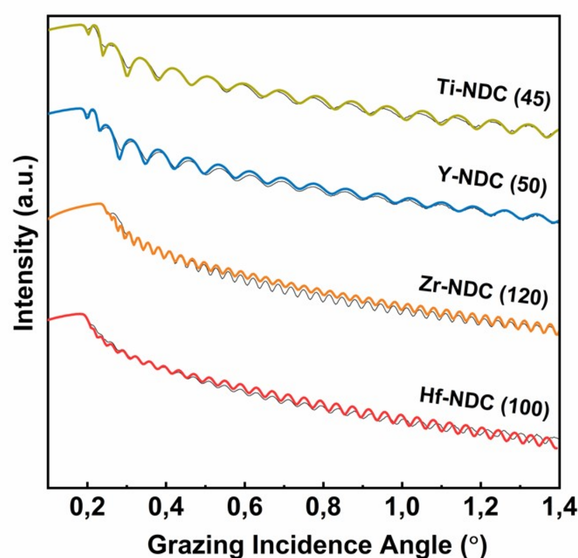

Fig. S1 XRR patterns for the as-deposited Ti-, Y-, Zr-, and Hf-NDC films with different total film thickness (nm). Black lines: measured data, colour lines: fitted patterns.

2. Fourier transform infrared spectroscopy (FTIR)

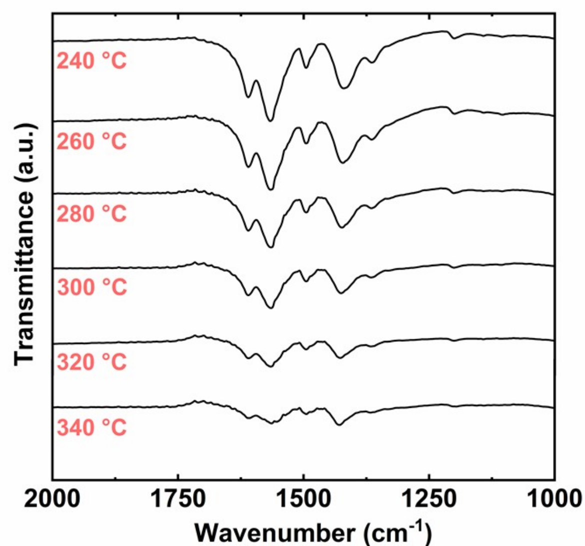

Fig. S2 FTIR reflection spectra of Y-NDC films deposited at different temperatures.

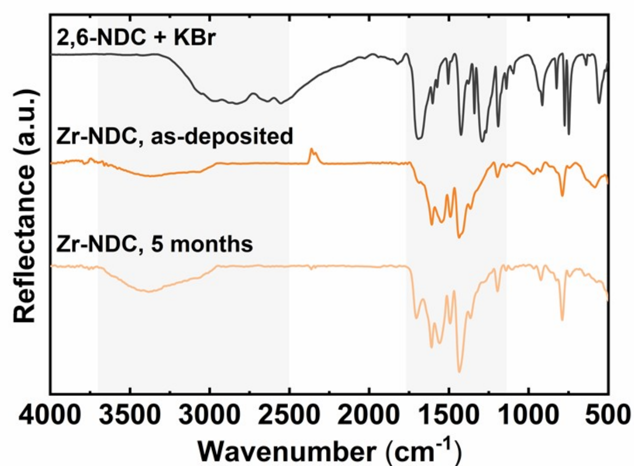

Fig. S3 FTIR reflection spectra of as-deposited Zr-NDC film and the same sample after 5 months of air-storage.

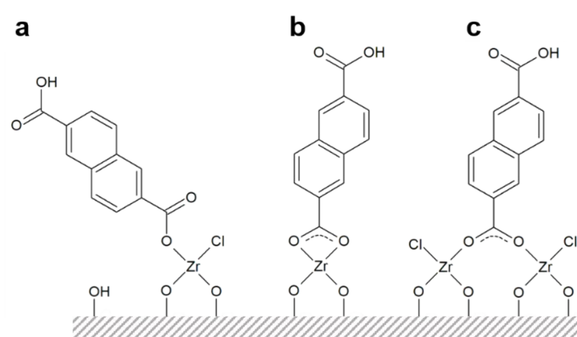

Fig. S4 Possible coordination modes of 2,6-NDC molecule to zirconium: **(a)** monodentate complex, **(b)** bidentate complex, and **(c)** bridging complex.

3. X-ray photoelectron spectroscopy (XPS)

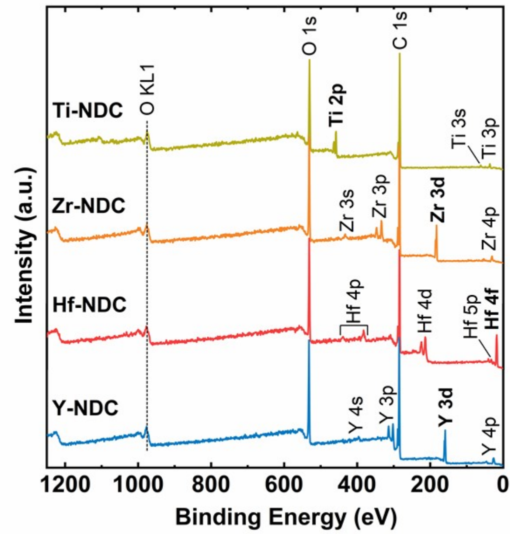

Fig. S5 XPS survey spectra for Ti-NDC, Zr-NDC, Hf-NDC and Y-NDC films.

4. UV-Vis and PL spectroscopy

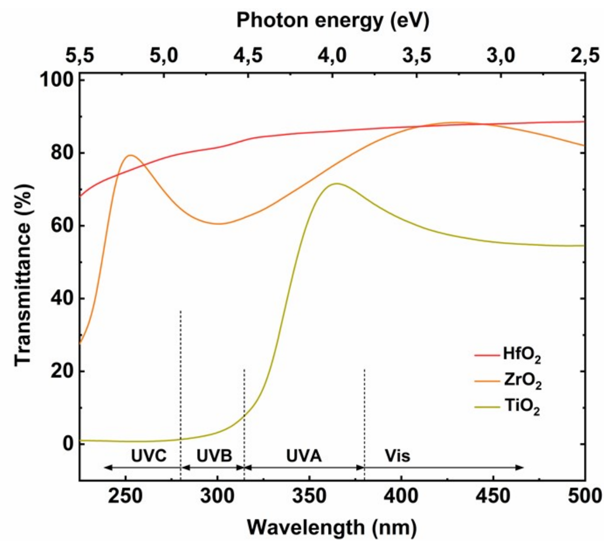

Fig. S6 UV-Vis transmission spectra for three deposited metal oxide thin films: TiO_2 (60 nm), ZrO_2 (101 nm) and HfO_2 (50 nm). The deposition parameters for HfO_2, ZrO_2 and TiO_2 were respectively: 0.4/0.5/0.5/0.5 for $HfCl_4$/purge/H_2O/purge at 300 °C; 3/6/5/6 for $ZrCl_4$/purge/H_2O/purge at 265 °C and 1/2/1/2 s for $TiCl_4$/purge/H_2O/purge at 300 °C.

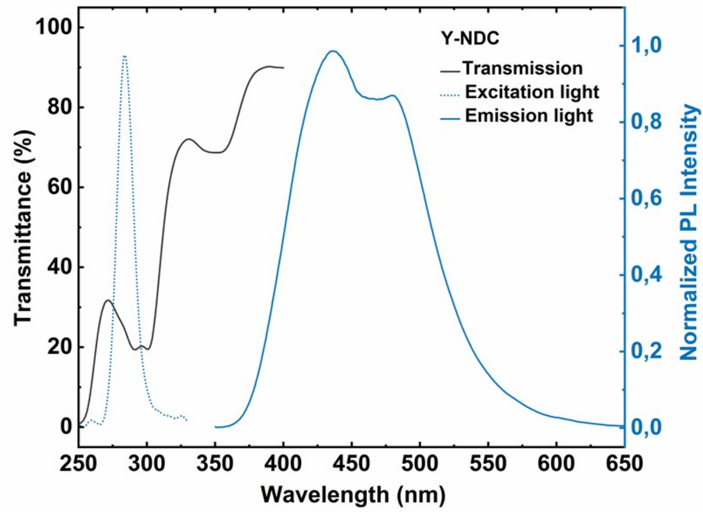

Fig. S7 The optical transmission and photoluminescence emission of the Y-NDC film (99 nm).

5. Fourier transform infrared spectroscopy (FTIR) after UV irradiation

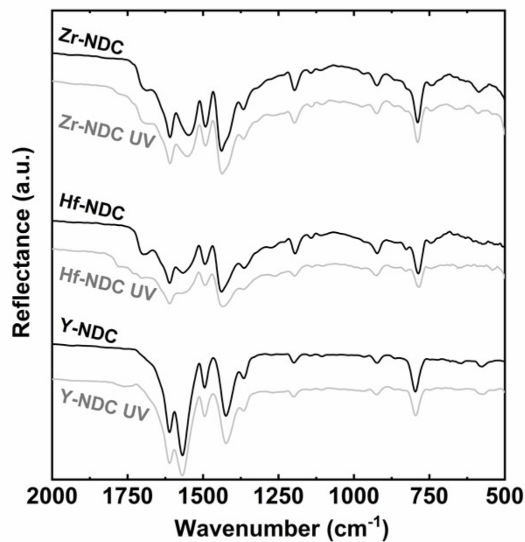

Fig. S8 FTIR reflection spectra of Zr-NDC, Hf-NDC and Y-NDC thin films before and after 3 hours of irradiation by 365 nm UV light. The photon flux was 2100 mW/cm^2 at a working distance of ~5 mm. Black lines: as-deposited films, grey lines: films after UV irradiation.

6. X-ray diffraction (XRD)

X-ray diffraction measurements were performed using Bruker AXS D8-A25 diffractometer equipped with a LynxEye strip detector and Ge (111) focusing monochromator, providing CuK_α radiation.

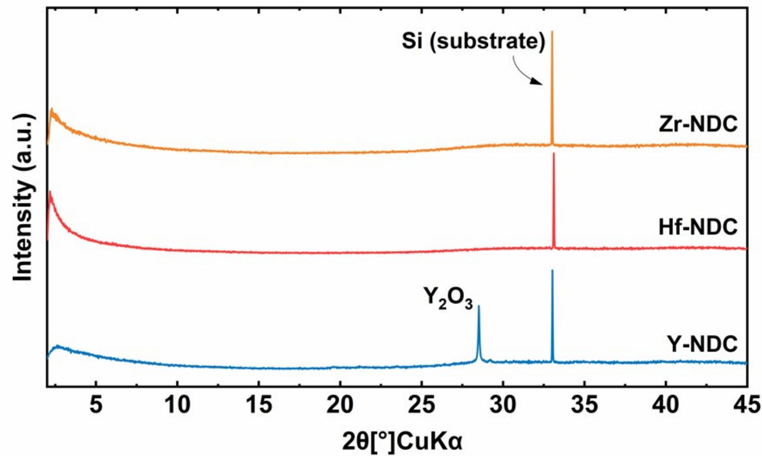

Fig. S9 X-ray diffractograms for the as-deposited Zr-NDC, Hf-NDC and Y-NDC samples.

7. Atomic force microscopy (AFM)

AFM measurements for Ti-NDC and Zr-NDC films were performed in noncontact mode with a scan size of 10 x 10 µm^2 and 256 px resolution using Park XE70 instrument from Park Systems. To scan Hf-NDC and Y-NDC films, we used JPK NanoWizard 4 Bioscience AFM in the Quantitative Imaging (QI™)-mode, with a ContAl-G cantilever (NanoSensors, k = 0.2 N/m and l = 450 µm). The off-resonance QI™ mode (with tip-sample vertical interaction force measured and recorded at each scanned pixel) was used to obtain surface topography and surface adhesion maps with a scan size of 10 x 10 µm^2 and 256 px resolution. Adhesion was probed in air at ambient conditions in a temperature-controlled box (25 ± 0.5 °C). The RMS roughness was calculated as an average value from three line profiles picked in three different regions on each scanned sample. The AFM images were processed using Gwyddion 2.56 software.

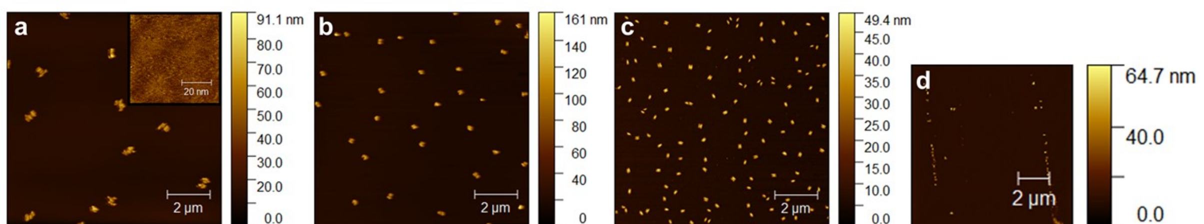

Fig. S10 Surface topography as measured by AFM for **(a)** Zr-NDC (110 nm), **(b)** Ti-NDC (99 nm), **(c)** Hf-NDC (93 nm) and **(d)** Y-NDC (102 nm). Zoomed-in image on **(a)** showing only flat surface without islands.

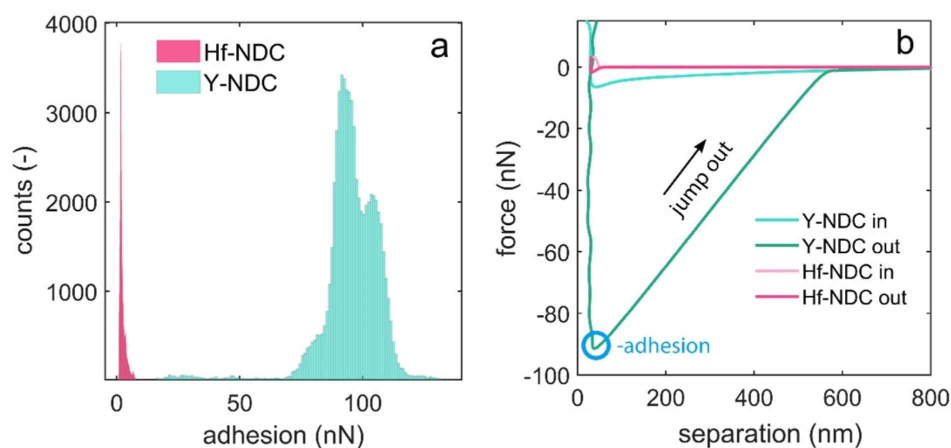

Fig. S11 Adhesion measured between an AFM tip and Hf-NDC or Y-NDC samples in air at ambient conditions: **(a)** histograms comparing the distribution of adhesion values for two films extracted from the measured adhesion maps with vertical force-distance curves measured at each scanned pixel (scan size 10 x 10 μm^2 and 256 px-resolution); **(b)** representative force-separation distance curves measured on approach (in) and on retraction (out). Adhesion shown in panel **(a)** was determined as the absolute minimum measured force before an adhesive jump-out event. The measured adhesion force for Hf-NDC was 2.3 ± 0.1 nN and for Y-NDC 95.1 ± 4.1 nN.

8. Stability test

Table S1 Film thickness before and after 24 hours of exposure to DI water as measured by SE

Sample	Initial thickness (nm)	Thickness after 24 hours (nm)
Ti-NDC	112.4	40.6
Zr-NDC	125.7	119.3
Hf-NDC	98.6	70.2
Y-NDC	107.7	2.1

9. Contact angle (CA) measurements

Contact angle measurements were performed using Theta Lite optical tensiometer from Biolin Scientific.

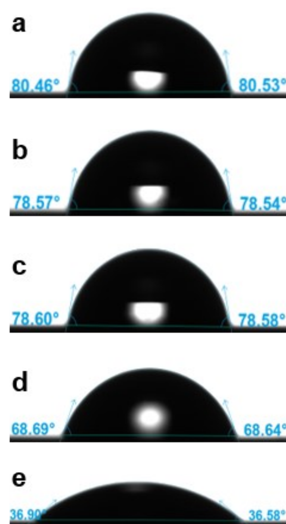

Fig. S12 Contact angle measurements between DI water and films: **(a)** Ti-NDC film (80°), **(b)** Hf-NDC film (78°), **(c)** Zr-NDC film (78°), **(d)** Y-NDC film (68°), and **(e)** precleaned Si substrate (36°).