Supporting Information:

Dye-sensitized polyoxometalate for visible-light-driven photoelectrochemical cells

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1. Crystal data of MoBB3.

Table S1. Crystal data and structure refinement for **MoBB3**.

Empirical formula	$C_{40}\ H_{52}\ Mo_6\ N_6\ O_{21}$
Formula weight	1528.52
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 10.9209(6) Å α= 90° b = 19.2268(13) Å β= 101.122(2)° c = 11.9644(7) Å γ = 90°
Volume	2465.0(3) $Å^3$
Z	2
Density (calculated)	2.059 Mg/m^3
Goodness of fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0256, wR2 = 0.0524
R indices (all data)	R1 = 0.0326, wR2 = 0.0548

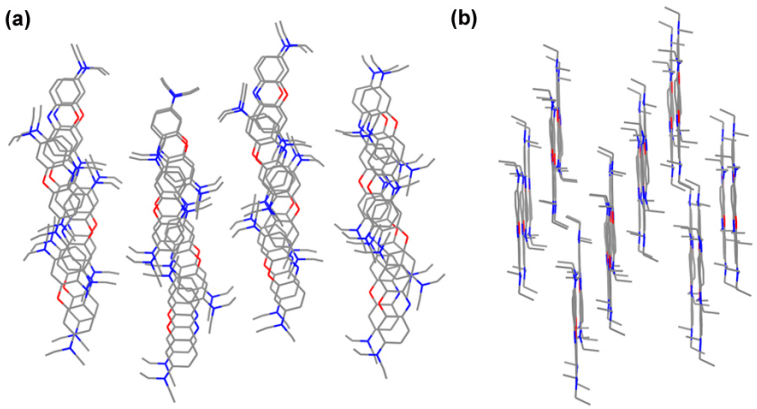

Figure S1. a) The alignment of dye cations in **MoBB3** along the z-axis. b) The alignment of dye cations in **MoBB3** along the y-axis.

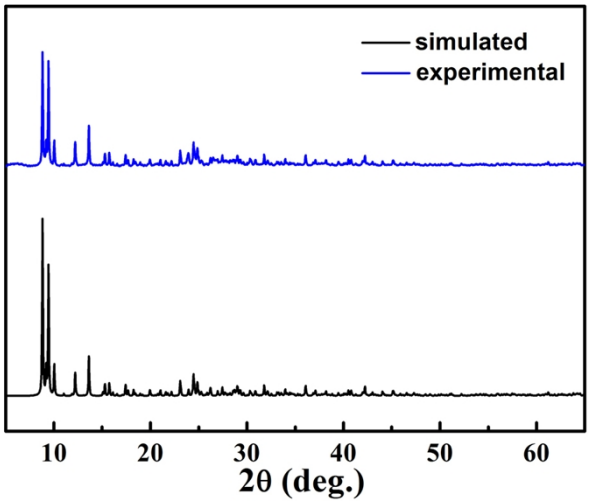

Figure S2. Simulated and experimental XRD patterns of **MoBB3**.

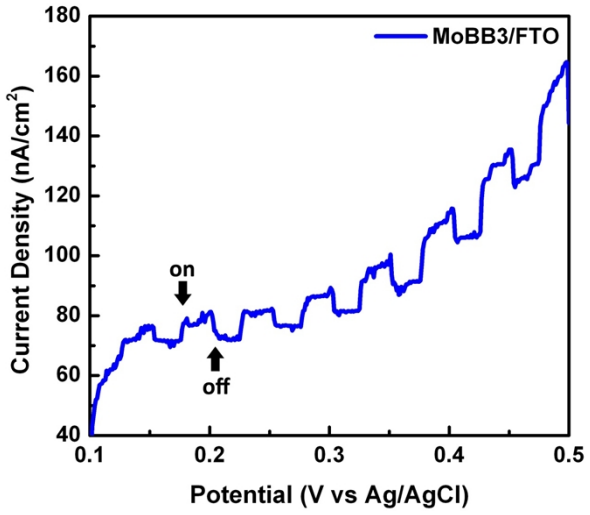

Figure S3. The photocurrent-voltage (J-V) behavior of **MoBB3**/FTO recorded using linear sweep voltammetry under chopped AM 1.5 G illumination.