Electronic Supplementary Material (ESI) for Dalton Transactions

Experimental and Theoretical Studies on Pyrene-grafted Polyoxometalate Hybrid

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Supporting Information:

1. Crytal data of MoAP.

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

Empirical formula	C_{48} H_{81} Mo_6 N_3 O_{18}
Formula weight	1563.80
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.3547(6) Å α= 78.355(2)° b = 12.8923(6) Å β= 78.467(2)° c = 19.6931(9) Å γ = 72.716(2)°
Volume	2900.4(2) $Å^3$
Z	2
Density (calculated)	1.791 Mg/m^3
Goodness of fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1323
R indices (all data)	R1 = 0.1463, wR2 = 0.1893

2. The photophysical properties of 1AP in acetonitrile

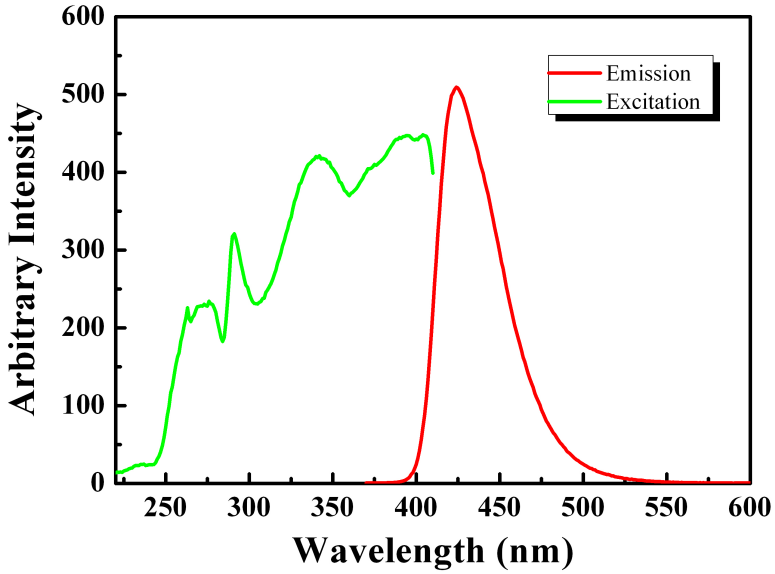

Figure S1. The excitation and emission spectra of **1AP** in acetonitrile at the concentration of $2.5*10^{-5}$ M.

3. The molecular orbital scaled energy diagrams of MoAP, 1AP and Mo_6O_{19}

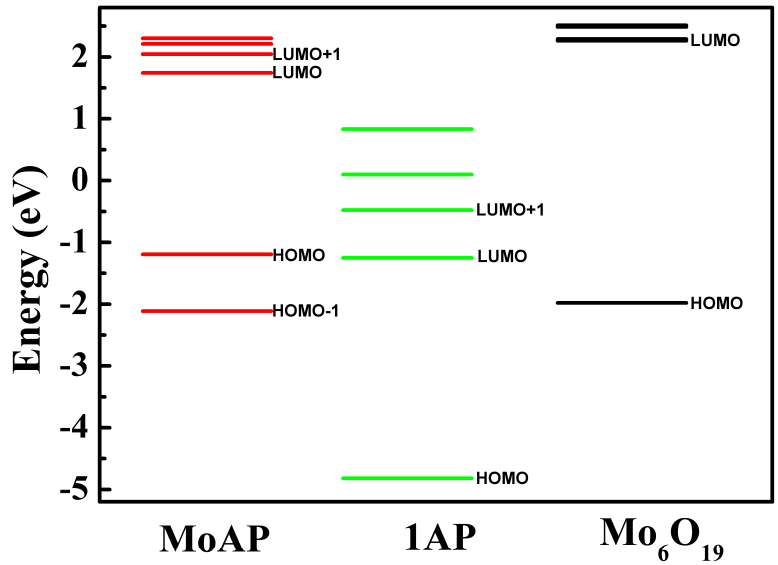

Figure S2. Molecular orbital scaled energy diagrams of **MoAP**, **1AP** and **Mo_6O_{19}**.