Supporting Information for

Two Dimensional Bicapped Supramolecular Hybrid Semiconductor Material Constructed from the Insulators *α*-Keggin Polyoxomolybdate and 4,4'-bipyridine

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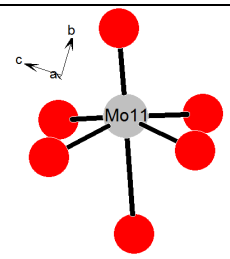
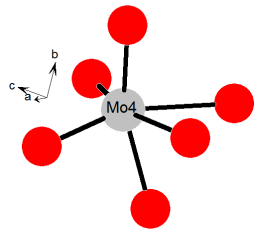
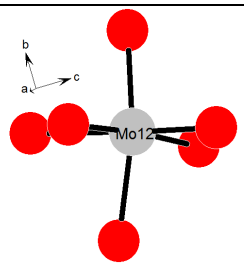
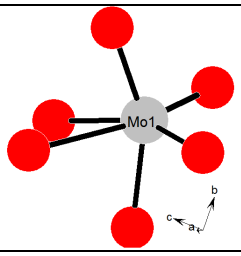
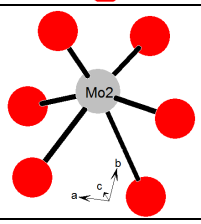
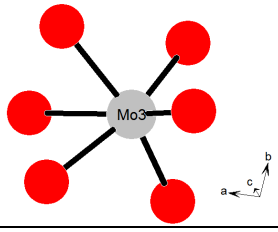
Tables

Table S1: The selected bond lengths and the coordination sphere of all the Mo atoms in $SiMo_{14}$-bpy_2

Central metal atom	Linked oxygen atom	Bond length	Average Bond length	Coordination sphere
Mo11	O39 O3 O38 O31 O17 O7	1.672 1.930 1.926 1.959 1.960 2.375	1.97	
Mo4	O37 025 O30 O24 O31 O7	1.687 1.834 1.971 2.145 1.861 2.375	1.98	
Mo12	O44 O36 O22 O30 O24 O15	1.708 1.720 1.996 2.169 2.004 2.193	1.96	
Mo1	O26 O8 O24 O15 O17 O7	1.690 1.846 2.136 1.934 1.854 2.364	1.97	
Mo2	O12 O9 O38 O29 O19 O13	1.859 1.685 1.840 2.119 1.974 2.379	1.97	
Mo3	O32 O13 O20 O8 O1 O12	1.682 2.353 1.956 1.961 1.917 1.948	1.96	

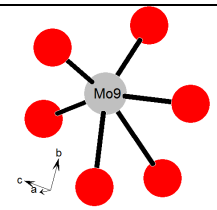
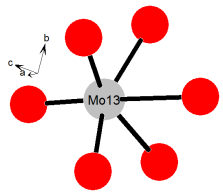
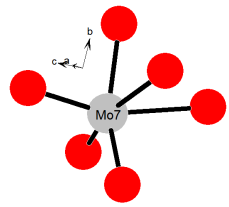
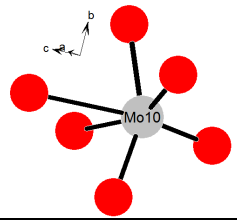
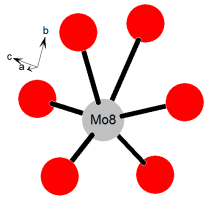
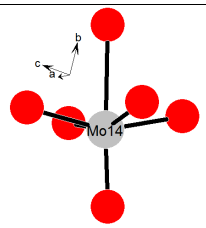
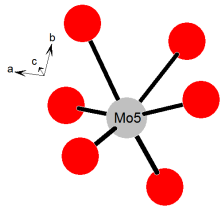
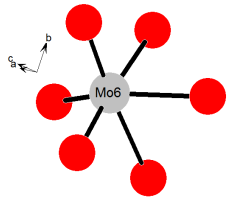
Mo9	O41 O21 O19 O23 O11 O3	1.686 1.836 1.955 2.117 2.376 1.852	1.97	
Mo13	O14 O35 O27 O25 O21 O11	1.949 1.683 1.959 1.949 1.934 2.390	1.97	
Mo7	O34 O27 O10 O22 O30 O18	1.681 1.829 1.863 2.124 1.950 2.359	1.96	
Mo10	O1 O28 O16 O15 O22 O18	1.851 1.680 1.848 1.957 2.150 2.362	1.97	
Mo8	O33 O2 O5 O23 O14 O11	1.687 1.938 1.821 2.157 1.854 2.356	1.97	
Mo14	O42 O10 O16 O5 O6 O18	1.686 1.961 1.948 1.941 1.949 2.379	1.96	
Mo5	O4 O6 O2 O29 O20 O13	1.682 1.853 1.940 2.127 1.857 2.349	1.96	
Mo6	O43 O40 O29 O19 O2 O23	1.712 1.716 2.021 2.128 2.208 2.005	1.96	

Table S2: The absorption frequencies for $SiMo_{14}$-bpy_2 and $SiMo_{12}$-bpy_3 within the range 1100-400 cm^{-1}

Vibrational Mode	**$[SiMo_{12}O_{40}](H4,4'\text{-}bpy)_3$ cm^{-1}**	**$[SiMo_{14}O_{44}](H_24,4'\text{-}bpy)_2$ cm^{-1}**
Mo-O_t	940 (s)	983 (m), 971 (w),953 (s)
Si-O_c	895 (w)	896 (s)
Mo-O_c-Mo edge sharing	857 (w)	878 (s), 848 (s)
Mo-O_b-Mo corner sharing	800 (s)	791 (s), 758 (m),683 (w)

Table S3: The XPS binding energies (eV) of Mo 3d in the sample $SiMo_{14}$-bpy_2

Peak value (eV)	**Intensity**	**Area**	**Spin-Orbit Component**
231.23 (4)	318.264	542.05	$3d_{5/2}$ (Mo^{+5})
232.62 (1)	1672.723	2855.77	$3d_{5/2}$ (Mo^{+6})
234.6 (2)	316.403	538.88	$3d_{3/2}$ (Mo^{+5})
235.72 (4)	1098.352	1870.65	$3d_{3/2}$ (Mo^{+6})

Figures

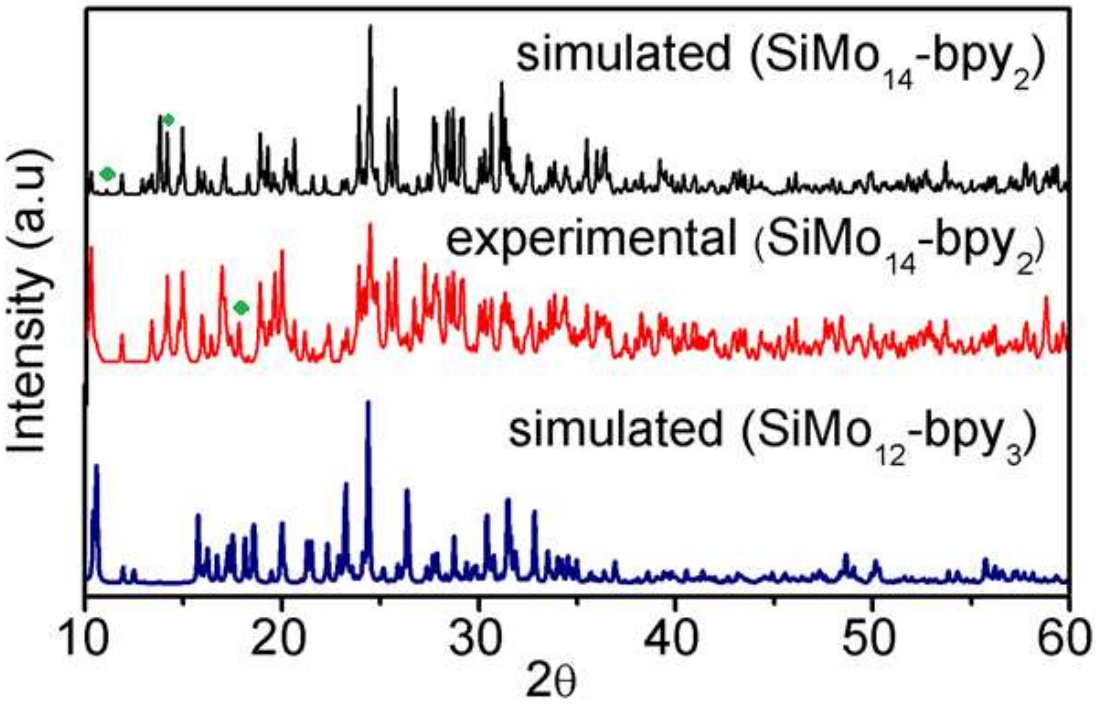


Figure S1: The pXRD comparison of the sample $SiMo_{14}$-bpy_2 with the simulated single crystal XRD of the sample $SiMo_{14}$-bpy_2 along with the simulated single crystal XRD pattern of $SiMo_{12}$-bpy_3. The peaks marked in green correspond to some of the unindexed peaks.

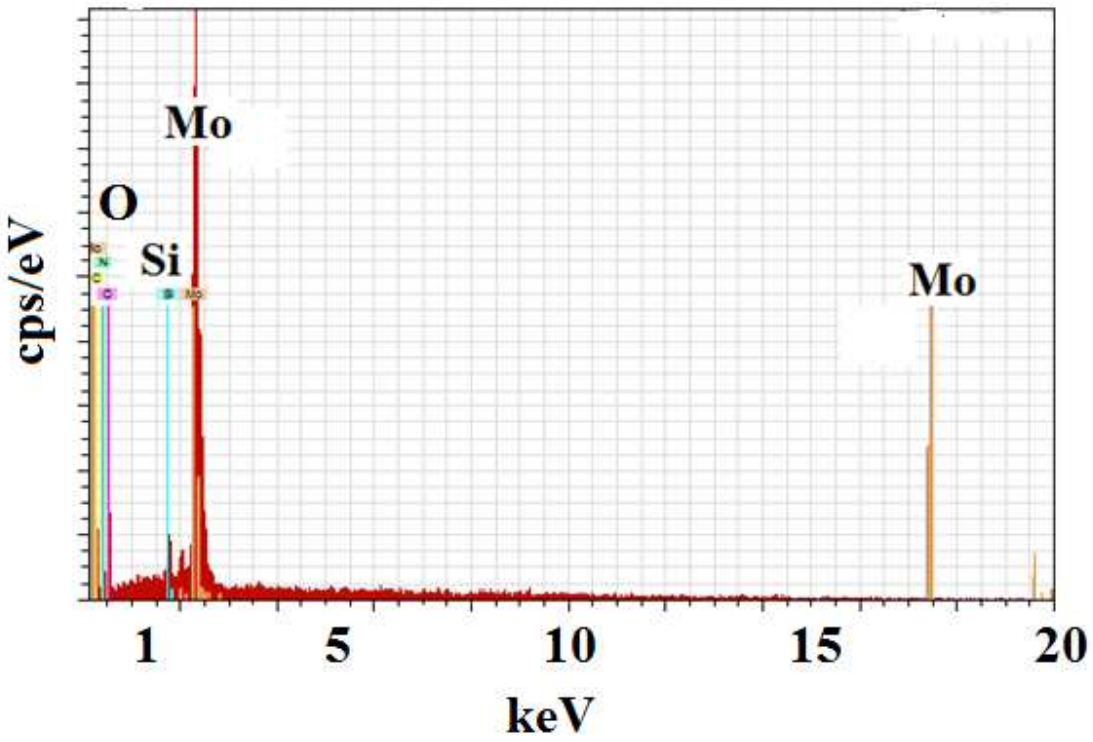


Figure S2: The EDAX spectrum of the $SiMo_{14}$-bpy_2.

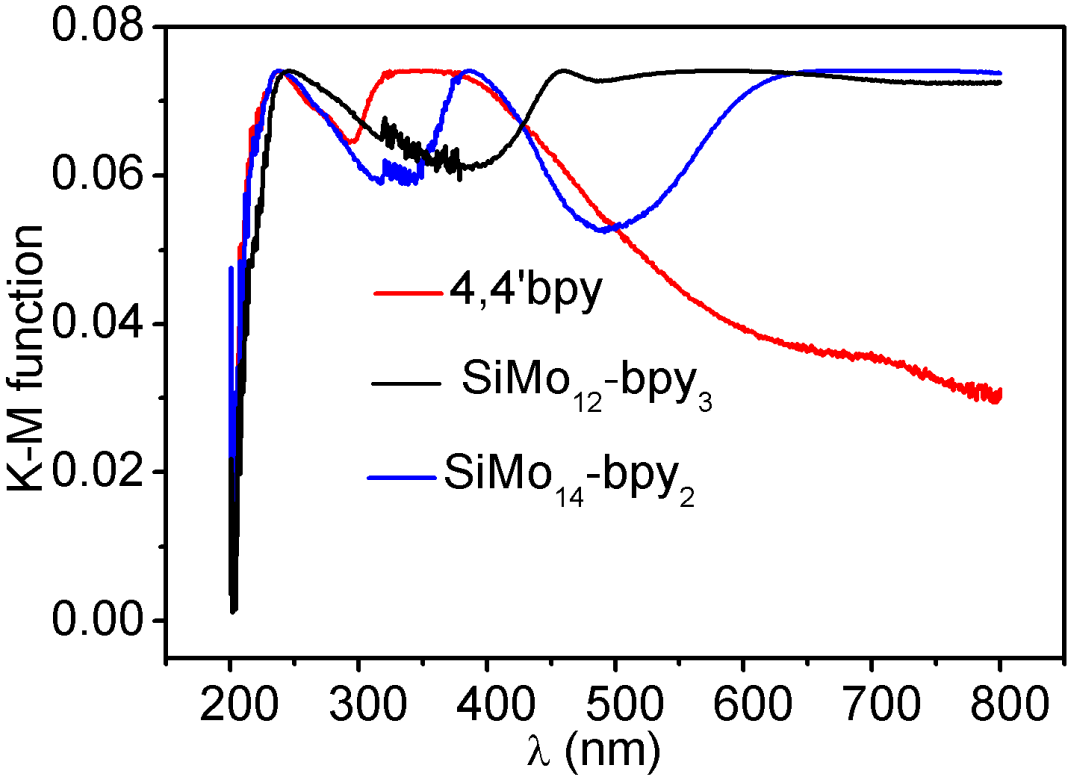


Figure S3: The diffused reflectance study fitted to the KM equation for the free 4,4'-bpy and hybrid materials $SiMo_{12}$-bpy_3 and $SiMo_{14}$-bpy_2 in the range 200-800 nm.

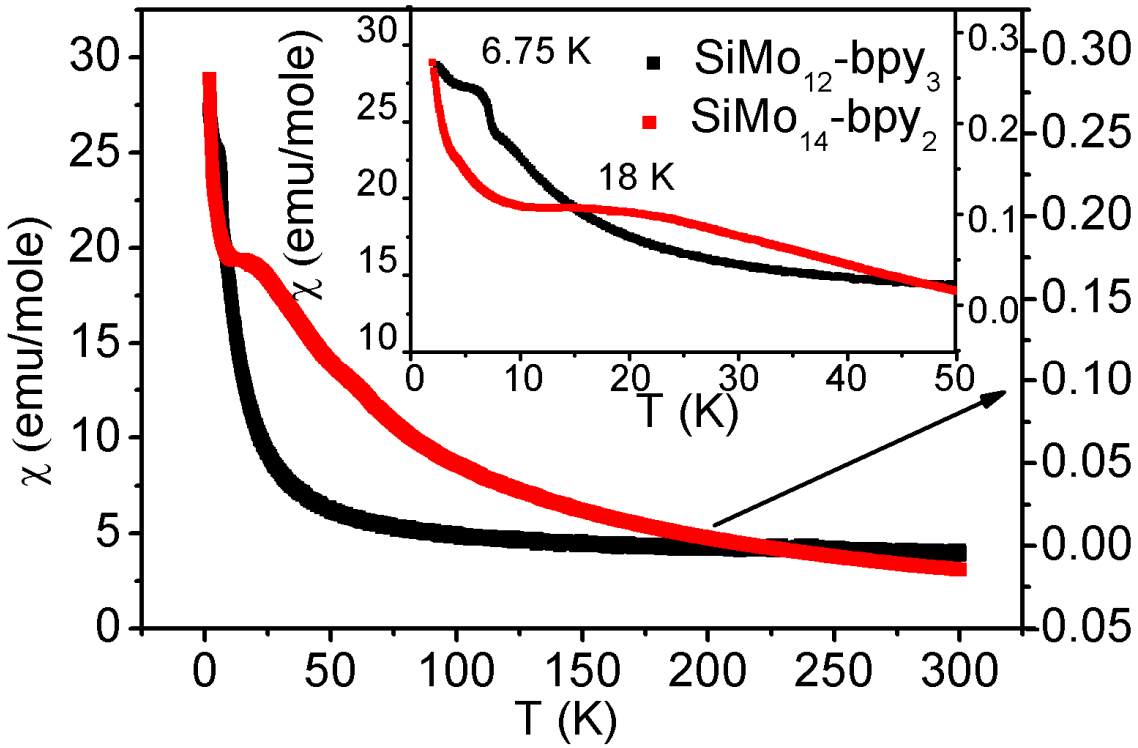


Figure S4: Temperature dependent magnetic susceptibility for the compounds $SiMo_{14}$-bpy_2 and $SiMo_{12}$-bpy_3 at 1000 Oe. The inset shows the low temperature region.