Structural, Electronic and Magnetic Properties of One Dimensional Organic Bimetal-Naphthalene Sandwich Nanowires (OBNSWs)

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Supporting Information

Table S1. Energy differences of different spin states of 1D $[Np_2V_2TM_2]_\infty$(TM=Ti, Cr, Mn, Fe) wires.

System		C(Å)	M	ΔE(eV)	Individual MMs (μ_B)				GS	
					V_1	V_2	TM_1	TM_2		
Isomer-□	V-Ti	7.15	1	0	0.994	-0.994	0.483	-0.483	AFM	Metal
			5	0.116	0.880	0.880	0.910	0.910		
			3	0.054	-0.461	0.667	0.749	0.779		
			7	0.272	1.696	1.696	1.005	1.005		
	V-Cr	6.82	3	0	0.873	0.873	0.204	0.204	FM	Metal
			1	0.076	-0.149	-0.161	0.150	0.150		
			5	0.115	1.390	1.390	0.717	0.728		
	V-Fe	6.94	7	0	1.450	1.450	1.787	1.787	FM	HM
			1	0.245	1.532	1.412	-1.663	-1.367		
			3	0.079	-0.749	-0.828	1.795	1.827		
			5	0.065	0.286	0.242	1.819	1.809		
			9	0.231	1.830	1.831	2.111	2.111		
	V-Mn	7.16	7	0	0.995	1.155	3.557	0.465	FM	HM
			3	0.131	-0.006	-1.429	3.027	0.432		
			5	0.184	0.397	-0.789	3.629	0.601		
			9	0.068	1.925	1.905	3.105	1.079		
			1	0.767	1.720	1.720	-1.862	-1.855		
Isomer-Ⅱ	V-Ti	7.2	3	0	0.921	0.919	0.094	0.075	FM	Metal
			5	0.457	0.936	0.939	0.946	0.945		

			1	0.254	0.029	-0.027	0.043	-0.044		
	V-Cr	6.89	3	0	0.929	0.930	0.058	0.058	FM	HM
			1	0.031	0	0	0	0		
			5	0.388	1.553	1.553	0.464	0.464		
	V-Fe	7.19	9	0	1.680	1.680	2.405	2.405	FM	SC
			7	0.175	0.871	0.880	2.333	2.333		
			5	0.245	-0.306	-0.306	2.433	2.433		
			3	0.613	-0.844	-0.836	2.173	2.168		
			11	0.694	2.105	2.103	2.618	2.618		
			1	0.117	-0.647	-0.763	1.382	0.425		
Isomer-III	V-Ti	7.25	1	0	1.324	-1.324	0.755	-0.755	AFM	Metal
			3	0.097	1.137	0.290	-0.502	0.951		
			5	0.217	0.847	0.501	1.152	1.016		
	V-Cr	7.05	5	0	-0.344	1.266	3.015	-0.077	FIM	HM
			1	0.124	-0.555	0.555	0.049	-0.049		
			3	0.135	0.776	0.759	0.348	0.336		
			7	0.126	1.168	1.312	3.131	0.265		

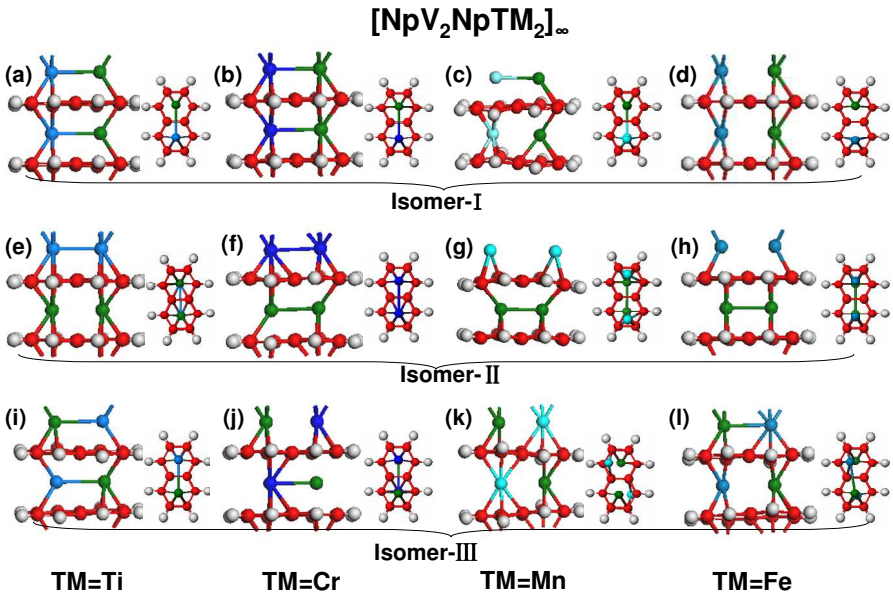

Figure S1. (a-l)Optimized structures of 1D $[Np_2V_2TM_2]_\infty$ OBNSWs.

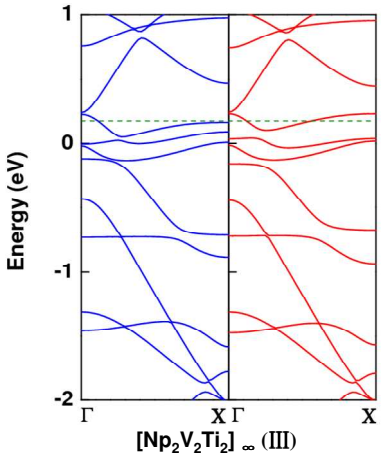

Figure S2. Band structures of 1D $[Np_2V_2Ti_2]_\infty$ at isomer-□.

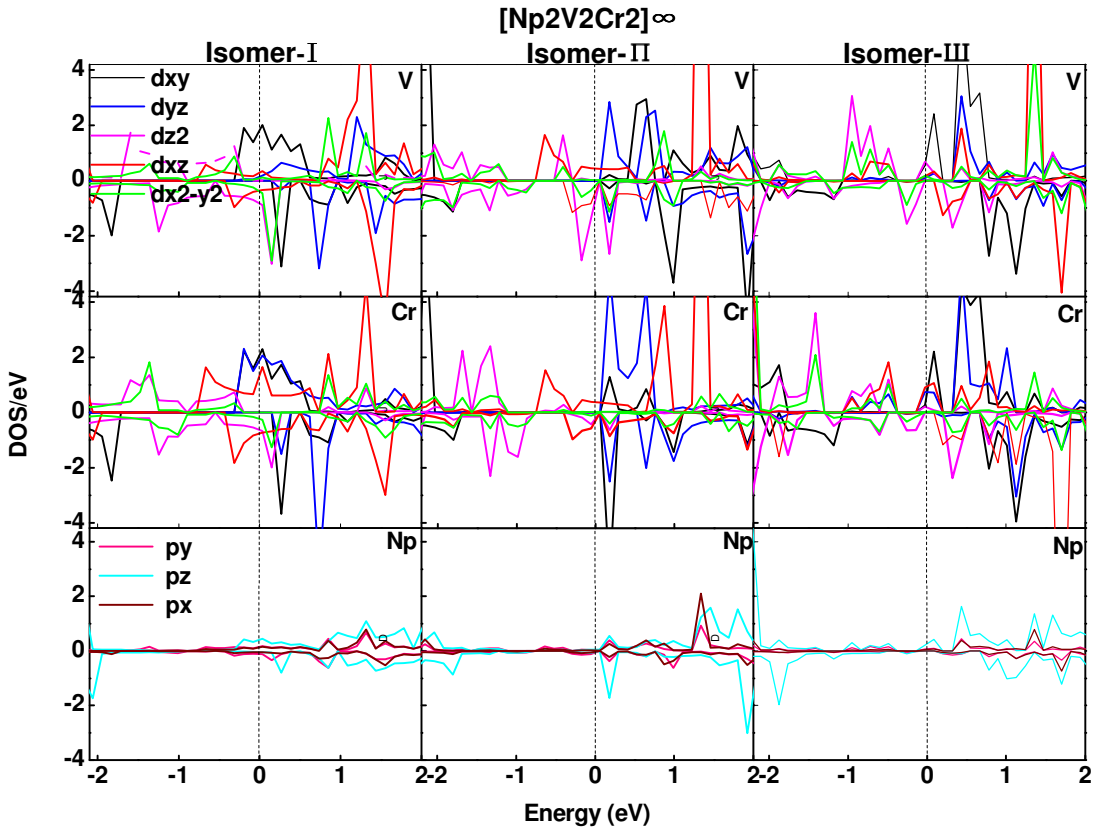

Figure S3. Local density of states (LDOS) of $[Np_2V_2Cr_2]_\infty$ (isomer- I,□,□).