Supporting information for:

Computational Screening of MN_4 (M = Ti - Cu) based Metal Organic Frameworks for CO_2 Reduction using d-band Centre as Descriptor

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Table S1. The lattice parameters and main bond lengths for MN_4-MOFs.

	TiN_4	VN_4	CrN_4	MnN_4	FeN_4	CoN_4	NiN_4	CuN_4
Lattice parameter (a=b) (Å)	22.65	22.23	22.11	22.02	21.98	21.84	21.82	21.80
M-N bonds (Å)	2.100 2.100 2.100 2.100	1.959 1.960 1.960 1.959	1.924 1.926 1.927 1.924	1.898 1.900 1.900 1.898	1.862 1.864 1.864 1.862	1.822 1.824 1.824 1.822	1.826 1.829 1.830 1.827	1.824 1.826 1.826 1.824

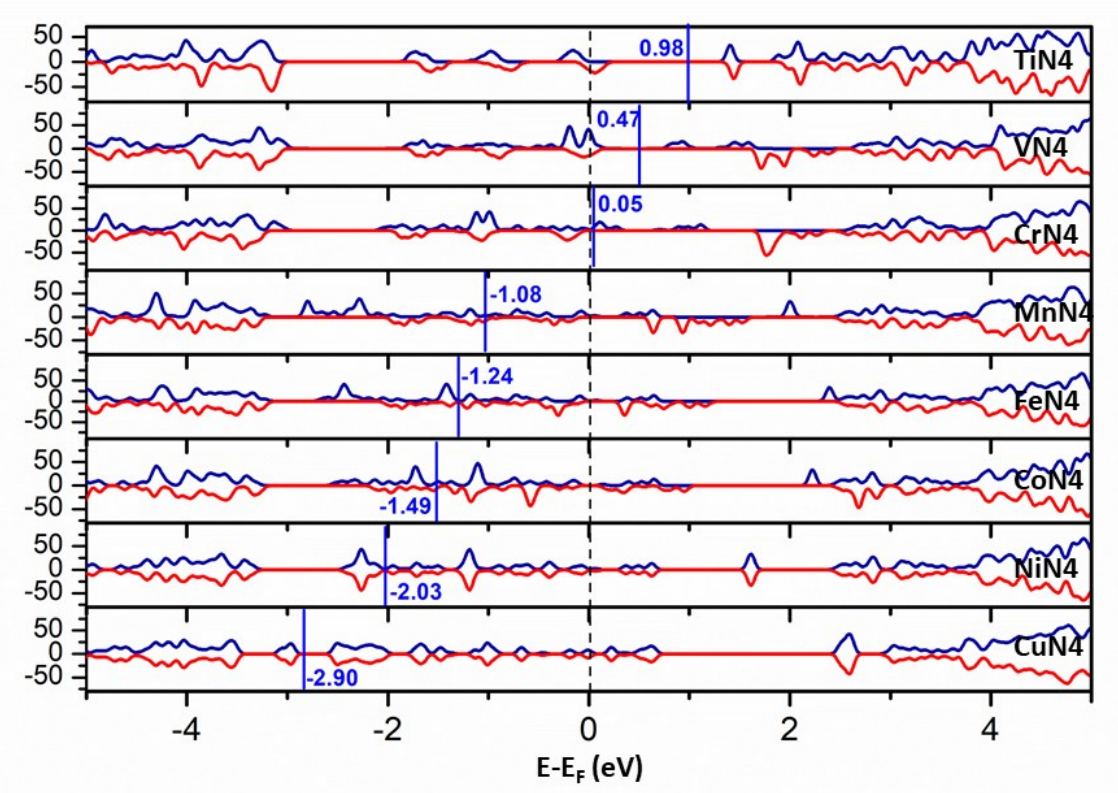

Figure S1. Projected density of states (PDOS) for 3d states of TM atoms in MN_4-MOFs. The vertical dash dotted lines correspond to the fermi level which is shifted to zero. The d-band centres are shown in blue vertical lines.

Table S2. The correction from ZPE and entropy used for TMN4-MOFs (Unit is eV).

species	ZPE	Entropy (-TS)
***CO**	0.22	-0.06
***COOH**	0.64	-0.15
***OCHO**	0.44	-0.10
***OCHOH**	0.82	-0.08
***OCH_2OH**	1.20	-0.13
***CHO**	0.48	-0.16
***OCH_2**	0.76	-0.07
***OCH_3**	1.08	-0.15
***CH_3OH**	1.35	-0.20
***OH**	0.40	-0.04
***H_2O**	0.66	-0.15