

Supplementary Information

Frist principle study for band engineering of KNbO₃ with 3d transition metal substitution

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Table S1. Pseudopotentials and ENMAX (eV) of all involved elements are listed for the clarification. The cutoff value is defined by 1.3 times O ENMAX according to the VASP manual.

Pseudopotentials	ENMAX
PAW_PBE K_sv 06Sep2000	259.264
PAW_PBE Ba_sv 06Sep2000	187.181
PAW_PBE Nb_sv 25May2007	293.235
PAW_PBE O 08Apr2002	400.000
PAW_PBE Ti_sv 26Sep2005	274.610
PAW_PBE V_sv 02Aug2007	263.673
PAW_PBE Cr_pv 02Aug2007	265.681
PAW_PBE Mn_pv 02Aug2007	269.864
PAW_PBE Fe 06Sep2000	267.882
PAW_PBE Co 02Aug2007	267.968
PAW_PBE Ni 02Aug2007	269.532
PAW_PBE Cu 22Jun2005	295.446
PAW_PBE Zn 06Sep2000	276.723

Table S2. Lattice lengths (Å), angles (°) and tetragonality (c/a) for all doped systems after structure relaxation.

	$a=b$	c	c/a	α	θ	γ
Ti	8.111	8.124	1.002	90.020	90.043	89.980
V	8.102	8.115	1.002	90.015	90.049	89.985
Cr	8.100	8.113	1.002	90.014	90.049	89.986
Mn	8.200	8.309	1.013	89.716	90.181	90.284
Fe	8.091	8.148	1.007	89.987	90.101	90.013
Co	8.177	8.228	1.006	89.836	90.219	90.164
Ni	8.168	8.218	1.006	89.843	90.171	90.157
Cu	8.184	8.243	1.007	89.808	90.184	90.192
Zn	8.186	8.285	1.012	89.752	90.189	90.248
KNbO ₃	8.057	8.057	1.000	90.000	90.000	90.000

Table S3. Summaries of electronic shell configuration, orbital arrangement and chemical valences for Ti ~ Zn doped systems obtained using Bader charge analysis (Plus sign for loss and negative for gain of valence electrons).

	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
B'	+2.14	+1.90	+1.59	+1.47	+1.35	+1.16	+1.17	+1.11	+1.29
Ba	+1.55	+1.57	+1.57	+1.58	+1.56	+1.58	+1.57	+1.58	+1.58
K	+0.81	+0.82	+0.82	+0.83	+0.82	+0.83	+0.82	+0.82	+0.83
Nb	+2.58	+2.61	+2.62	+2.62	+2.62	+2.62	+2.63	+2.63	+2.63
O	-1.21	-1.21	-1.20	-1.19	-1.18	-1.18	-1.19	-1.18	-1.19