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|
| KNbO₃ | 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 |