

Supplementary material for tP16 article

Table S1: Calculated lattice constants (\AA) in pure 3d-transition metal X and ruthenium.

Transition metals	Lattice constants \AA
Sc	3.41 3.31 ^{exp} [1]
Ti	2.99 2.95 ^{exp} [1]
V	3.03 3.03 ^{exp} [1]
Cr	2.845 2.851 ^{theo} [2] 2.88 ^{exp} [3]
Mn	8.91 8.91 ^{exp} [1]
Fe	2.88 2.87 ^{exp} [1]
Co	2.51 2.51 ^{exp} [1]
Ni	3.53 3.52 ^{exp} [1]
Cu	3.64 3.61 ^{exp} [1]
Zn	2.63
Ru	2.71 2.71 ^{exp} [1]

[1] Introduction to Solid State Physics Charles Kittel, 2005.

[2] M.M. Tibane, Phase stability study of Pt-Cr and Ru-Cr binary alloys, (2011).

[3] S. Hong, C.L. Fu, Phase stability and elastic moduli of Cr₂Nb by first-principles calculations, Intermetallics (Barking) 7 (1999) 5–9.

Table S2: Calculated lattice constants and magnetic moments in pure chromium, ruthenium and iron for different values of Hubbard U parameter.

Cr		
U-Parameter (eV)	Lattice parameter (\AA)	Magnetic moments (μ_B)
0	2.848052	0.002
1	2.844156	0.012
1.5	2.842541	0.005
2.0	2.844156	0.025
2.5	2.840457	0.024
3.0	3.60161	4.94311
3.5	3.62143	4.99052
4.0	3.633813	5.00475

4.5	3.648309	5.032
Ru		
U-Parameter (eV)	Lattice parameter (Å)	Magnetic moments (μ_B)
0	2.71507	0
1	2.70756	0
1.5	2.707503	0
2.0	2.703801	0
2.5	2.70008	0
3.0	2.696155	0.04
3.5	2.692593	0.04
4.0	2.689075	0.04
4.5	2.683845	0
Fe		
U-Parameter (eV)	Lattice parameter (Å)	Magnetic moments (μ_B)
0	2.812846	0.0
1	2.851423	2.52474
1.5	2.861893	2.59111
2.0	2.866878	2.612445
2.5	2.871924	2.626665
3.0	2.880103	2.65511
3.5	2.887744	2.669335
4.0	2.899194	2.701925
4.5	2.910362	2.706665