Supporting Information

Data-Driven Deep Generative Design of Stable Spintronic Materials

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Supplementary Note 1: The Elemental and Electronic Properties for Feature Engineering

The following atomic and electronic properties were considered to develop the machine learning models. Here, BCC indicates body-centered cubic, and FCC means face-centered cubic.

Atomic volume	Is Mendeleev	Column number
Atomic number	Is meta	Covalent radius
Atomic weight	Is nonmetal	Density
BCC energy diff	Is metalloid	First ionization energy
BCC effective lattice constant	Is alkali	Ground state band gap
BCC fermi	Is d-block	Ground state efflatcnt
BCC magnetic moment	Is f-block	Ground state estBCClatcnt
BCC volume padiff	Number of valence	Ground state estFCClatcnt
BCC volume pa.	Number of unfilled	Ground state magnetic moment
Boiling temperature	Number of s valance	Ground state volume pa
ICSD volume	Space group number	Row number
Number of d unfilled	Number of d valence	Number of f unfilled
Number of f valence	Number of p unfilled	Number of p valence
Number of s unfilled	Oxidation states	Polarizability

Supplementary Note 2: Predicted Spintronic Materials

The following table contains the chemical formulas of the spintronic materials predicted by the deep neural network (DNN) model. The material structures can be downloaded from the Carolina Materials database at `http://www.carolinamatdb.org/`.

Supplementary Table 1: The spintronic materials predicted by the DNN model

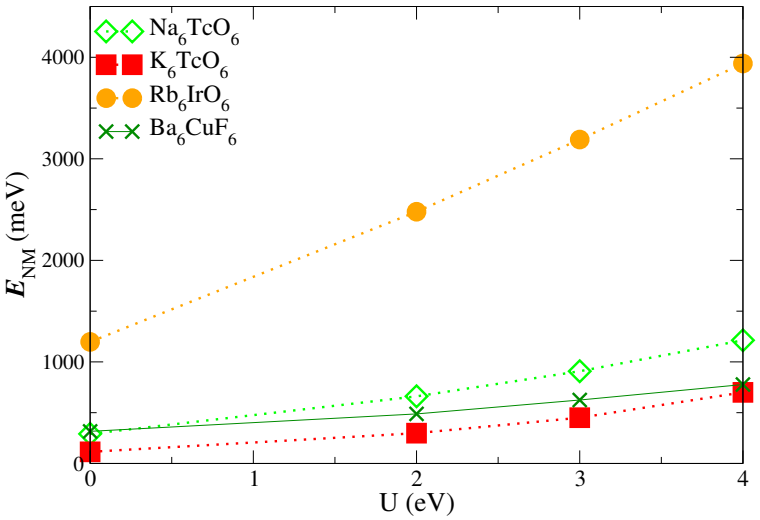
$AlCo_6N$	Fe_6RhCl	Fe_6N_6Cl
$BaCuF_6$	Fe_6RhN	Hf_6MnN_6
$BaNiF_6$	Fe_6RhS	K_6FeO_6
$BaRhF_6$	$FeCo_6C$	K_6OsS_6
$BaRuF_6$	$FeRh_6O$	K_6TcO_6
$CaCo_6N$	$GaCo_6N$	K_6WO_6
Co_6IrN	$HfCo_6C$	Mg_6FeO_6
Co_6RhN	$InCo_6N$	Na_6MoO_6
Co_6RuN	Mn_6AuS	Na_6RuO_6
Co_6SbN	$MnNi_6N$	Na_6TcO_6
Co_6TeO	$SrCuF_6$	Na_6WO_6
$CoNi_6N$	$TlCo_6P$	Rb_6IrO_6
Fe_6CoN	$ZrCo_6Cl$	Rb_6ReS_6
Fe_6PtCl	Cs_6ReS_6	Rb_6TcO_6
Fe_6PtN	Cs_6RuO_6	V_6S_6Cl

Supplementary Note 3: GGA and GGA+U Calculations

We performed GGA+U calculations to determine whether the onsite Coulomb potential affects the results. Table 2 contains the band gap values in eV for spin-up and spin-down electrons. It is clear that $BaCuF_6$ and Na_6TcO_6 remain half-metals. K6TcO6 and Rb_6IrO_6 have negligible band gap openings when we enable the U potential. Figure 1 shows the energy of the non-magnetic phase (E_{NM}) relative to the ferromagnetic phase as the U value is altered. The positive E_{NM} values indicate that all materials remain magnetic based on GGA+U calculations.

Supplementary Table 2: Band gap from GGA ($U = 0$ eV), and GGA+U calculations, when $U = 2$ eV and $U = 4$ eV.

Material	$U = 0$ eV		$U = 2$ eV		$U = 4$ eV	
	Up	Down	Up	Down	Up	Down
$BaCuF_6$	0.00	0.96	0.00	1.05	0.00	1.15
Na_6TcO_6	0.00	1.83	0.00	2.02	0.00	2.04
K_6TcO_6	0.00	0.00	0.00	0.03	0.00	0.02
Rb_6IrO_6	0.00	0.00	0.01	0.01	0.07	0.007



Supplementary Figure 1: The energy of non magnetic phase relative to the ferromagnetic phase based on GGA ($U = 0$) and GGA+U calculations.

Supplementary Note 4: Stable Structures

The following structures are the computationally discovered stable spintronic materials in the CIF format.

$BaCuF_6$

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'Ba4 Cu4 F24                                '
_cell_length_a                         8.125344
_cell_length_b                         8.125344
_cell_length_c                         8.125344
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           536.445139
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Ba1        1.0     0.750000     0.250000     0.750000    Biso  1.000000 Ba
   Ba2        1.0     0.750000     0.750000     0.250000    Biso  1.000000 Ba
   Ba3        1.0     0.250000     0.250000     0.250000    Biso  1.000000 Ba
   Ba4        1.0     0.250000     0.750000     0.750000    Biso  1.000000 Ba
   Cu1        1.0     -0.000000     -0.000000     -0.000000    Biso  1.000000 Cu
   Cu2        1.0     -0.000000     0.500000     0.500000    Biso  1.000000 Cu
   Cu3        1.0     0.500000     -0.000000     0.500000    Biso  1.000000 Cu
   Cu4        1.0     0.500000     0.500000     -0.000000    Biso  1.000000 Cu
   F1         1.0     0.500000     -0.000000     0.728783    Biso  1.000000 F
```

```
F2          1.0     0.500000     -0.000000     0.271217    Biso  1.000000 F
F3          1.0     0.228783     -0.000000     -0.000000    Biso  1.000000 F
F4          1.0     0.771217     -0.000000     -0.000000    Biso  1.000000 F
F5          1.0     -0.000000     0.228783     -0.000000    Biso  1.000000 F
F6          1.0     0.500000     0.271217     -0.000000    Biso  1.000000 F
F7          1.0     0.500000     0.500000     0.228783    Biso  1.000000 F
F8          1.0     0.500000     0.500000     0.771217    Biso  1.000000 F
F9          1.0     0.228783     0.500000     0.500000    Biso  1.000000 F
F10         1.0     0.771217     0.500000     0.500000    Biso  1.000000 F
F11         1.0     -0.000000     0.728783     0.500000    Biso  1.000000 F
F12         1.0     0.500000     0.771217     0.500000    Biso  1.000000 F
F13         1.0     -0.000000     -0.000000     0.228783    Biso  1.000000 F
F14         1.0     -0.000000     -0.000000     0.771217    Biso  1.000000 F
F15         1.0     0.728783     -0.000000     0.500000    Biso  1.000000 F
F16         1.0     0.271217     -0.000000     0.500000    Biso  1.000000 F
F17         1.0     0.500000     0.228783     0.500000    Biso  1.000000 F
F18         1.0     -0.000000     0.271217     0.500000    Biso  1.000000 F
F19         1.0     -0.000000     0.500000     0.728783    Biso  1.000000 F
F20         1.0     -0.000000     0.500000     0.271217    Biso  1.000000 F
F21         1.0     0.728783     0.500000     -0.000000    Biso  1.000000 F
F22         1.0     0.271217     0.500000     -0.000000    Biso  1.000000 F
F23         1.0     0.500000     0.728783     -0.000000    Biso  1.000000 F
F24         1.0     -0.000000     0.771217     -0.000000    Biso  1.000000 F
```

Na_6TcO_6

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'Na24 Tc4 O24                          '
_cell_length_a                         9.275142
_cell_length_b                         9.275142
_cell_length_c                         9.275142
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           797.924246
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Na1        1.0     -0.000000     0.750000     0.750000    Biso  1.000000 Na
   Na2        1.0     0.250000     -0.000000     0.750000    Biso  1.000000 Na
   Na3        1.0     -0.000000     0.250000     0.750000    Biso  1.000000 Na
   Na4        1.0     0.750000     -0.000000     0.750000    Biso  1.000000 Na
   Na5        1.0     0.250000     0.750000     -0.000000    Biso  1.000000 Na
   Na6        1.0     0.250000     0.250000     -0.000000    Biso  1.000000 Na
   Na7        1.0     -0.000000     0.250000     0.250000    Biso  1.000000 Na
   Na8        1.0     0.250000     0.500000     0.250000    Biso  1.000000 Na
   Na9        1.0     -0.000000     0.750000     0.250000    Biso  1.000000 Na
   Na10       1.0     0.750000     0.500000     0.250000    Biso  1.000000 Na
   Na11       1.0     0.250000     0.250000     0.500000    Biso  1.000000 Na
   Na12       1.0     0.250000     0.750000     0.500000    Biso  1.000000 Na
```

Na13	1.0	0.500000	0.750000	0.250000	Biso	1.000000 Na
Na14	1.0	0.750000	-0.000000	0.250000	Biso	1.000000 Na
Na15	1.0	0.500000	0.250000	0.250000	Biso	1.000000 Na
Na16	1.0	0.250000	-0.000000	0.250000	Biso	1.000000 Na
Na17	1.0	0.750000	0.750000	0.500000	Biso	1.000000 Na
Na18	1.0	0.750000	0.250000	0.500000	Biso	1.000000 Na
Na19	1.0	0.500000	0.250000	0.750000	Biso	1.000000 Na
Na20	1.0	0.750000	0.500000	0.750000	Biso	1.000000 Na
Na21	1.0	0.500000	0.750000	0.750000	Biso	1.000000 Na
Na22	1.0	0.250000	0.500000	0.750000	Biso	1.000000 Na
Na23	1.0	0.750000	0.250000	-0.000000	Biso	1.000000 Na
Na24	1.0	0.750000	0.750000	-0.000000	Biso	1.000000 Na
Tc1	1.0	-0.000000	-0.000000	-0.000000	Biso	1.000000 Tc
Tc2	1.0	-0.000000	0.500000	0.500000	Biso	1.000000 Tc
Tc3	1.0	0.500000	-0.000000	0.500000	Biso	1.000000 Tc
Tc4	1.0	0.500000	0.500000	-0.000000	Biso	1.000000 Tc
O1	1.0	0.500000	-0.000000	0.710815	Biso	1.000000 O
O2	1.0	-0.000000	-0.000000	0.789185	Biso	1.000000 O
O3	1.0	0.210815	-0.000000	-0.000000	Biso	1.000000 O
O4	1.0	0.789185	-0.000000	-0.000000	Biso	1.000000 O
O5	1.0	0.500000	0.710815	-0.000000	Biso	1.000000 O
O6	1.0	0.500000	0.289185	-0.000000	Biso	1.000000 O
O7	1.0	0.500000	0.500000	0.210815	Biso	1.000000 O
O8	1.0	-0.000000	0.500000	0.289185	Biso	1.000000 O
O9	1.0	0.210815	0.500000	0.500000	Biso	1.000000 O
O10	1.0	0.789185	0.500000	0.500000	Biso	1.000000 O
O11	1.0	0.500000	0.210815	0.500000	Biso	1.000000 O
O12	1.0	0.500000	0.789185	0.500000	Biso	1.000000 O
O13	1.0	-0.000000	-0.000000	0.210815	Biso	1.000000 O
O14	1.0	0.500000	-0.000000	0.289185	Biso	1.000000 O
O15	1.0	0.710815	-0.000000	0.500000	Biso	1.000000 O
O16	1.0	0.289185	-0.000000	0.500000	Biso	1.000000 O
O17	1.0	-0.000000	0.710815	0.500000	Biso	1.000000 O
O18	1.0	-0.000000	0.289185	0.500000	Biso	1.000000 O
O19	1.0	-0.000000	0.500000	0.710815	Biso	1.000000 O
O20	1.0	0.500000	0.500000	0.789185	Biso	1.000000 O
O21	1.0	0.710815	0.500000	-0.000000	Biso	1.000000 O
O22	1.0	0.289185	0.500000	-0.000000	Biso	1.000000 O
O23	1.0	-0.000000	0.210815	-0.000000	Biso	1.000000 O
O24	1.0	-0.000000	0.789185	-0.000000	Biso	1.000000 O

K_6TcO_6

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'K24 Tc O24                              '
_cell_length_a                         10.335238
_cell_length_b                         10.335238
_cell_length_c                         10.335238
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           1103.980452
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   K1         1.0     -0.000000     0.750000     0.750000    Biso  1.000000 K
   K2         1.0     0.250000     0.000000     0.750000    Biso  1.000000 K
   K3         1.0     -0.000000     0.250000     0.750000    Biso  1.000000 K
   K4         1.0     0.750000     -0.000000     0.750000    Biso  1.000000 K
   K5         1.0     0.250000     0.750000     0.000000    Biso  1.000000 K
   K6         1.0     0.250000     0.250000     0.000000    Biso  1.000000 K
   K7         1.0     -0.000000     0.250000     0.250000    Biso  1.000000 K
   K8         1.0     0.250000     0.500000     0.250000    Biso  1.000000 K
   K9         1.0     -0.000000     0.750000     0.250000    Biso  1.000000 K
   K10        1.0     0.750000     0.500000     0.250000    Biso  1.000000 K
   K11        1.0     0.250000     0.250000     0.500000    Biso  1.000000 K
   K12        1.0     0.250000     0.750000     0.500000    Biso  1.000000 K
   K13        1.0     0.500000     0.750000     0.250000    Biso  1.000000 K
```

```
K14         1.0     0.750000     0.000000     0.250000    Biso  1.000000 K
K15         1.0     0.500000     0.250000     0.250000    Biso  1.000000 K
K16         1.0     0.250000    -0.000000     0.250000    Biso  1.000000 K
K17         1.0     0.750000     0.750000     0.500000    Biso  1.000000 K
K18         1.0     0.750000     0.250000     0.500000    Biso  1.000000 K
K19         1.0     0.500000     0.250000     0.750000    Biso  1.000000 K
K20         1.0     0.750000     0.500000     0.750000    Biso  1.000000 K
K21         1.0     0.500000     0.750000     0.750000    Biso  1.000000 K
K22         1.0     0.250000     0.500000     0.750000    Biso  1.000000 K
K23         1.0     0.750000     0.250000     0.000000    Biso  1.000000 K
K24         1.0     0.750000     0.750000     0.000000    Biso  1.000000 K
Tc1         1.0    -0.000000    -0.000000     0.000000    Biso  1.000000 Tc
Tc2         1.0    -0.000000     0.500000     0.500000    Biso  1.000000 Tc
Tc3         1.0     0.500000    -0.000000     0.500000    Biso  1.000000 Tc
Tc4         1.0     0.500000     0.500000     0.000000    Biso  1.000000 Tc
O1          1.0     0.500000     0.000000     0.689645    Biso  1.000000 O
O2          1.0    -0.000000    -0.000000     0.810355    Biso  1.000000 O
O3          1.0     0.189645    -0.000000     0.000000    Biso  1.000000 O
O4          1.0     0.810355     0.000000     0.000000    Biso  1.000000 O
O5          1.0     0.500000     0.689645    -0.000000    Biso  1.000000 O
O6          1.0     0.500000     0.310355     0.000000    Biso  1.000000 O
O7          1.0     0.500000     0.500000     0.189645    Biso  1.000000 O
O8          1.0    -0.000000     0.500000     0.310355    Biso  1.000000 O
O9          1.0     0.189645     0.500000     0.500000    Biso  1.000000 O
O10         1.0     0.810355     0.500000     0.500000    Biso  1.000000 O
O11         1.0     0.500000     0.189645     0.500000    Biso  1.000000 O
O12         1.0     0.500000     0.810355     0.500000    Biso  1.000000 O
O13         1.0    -0.000000     0.000000     0.189645    Biso  1.000000 O
O14         1.0     0.500000    -0.000000     0.310355    Biso  1.000000 O
O15         1.0     0.689645    -0.000000     0.500000    Biso  1.000000 O
O16         1.0     0.310355     0.000000     0.500000    Biso  1.000000 O
O17         1.0    -0.000000     0.689645     0.500000    Biso  1.000000 O
O18         1.0    -0.000000     0.310355     0.500000    Biso  1.000000 O
O19         1.0    -0.000000     0.500000     0.689645    Biso  1.000000 O
O20         1.0     0.500000     0.500000     0.810355    Biso  1.000000 O
O21         1.0     0.689645     0.500000    -0.000000    Biso  1.000000 O
O22         1.0     0.310355     0.500000    -0.000000    Biso  1.000000 O
O23         1.0    -0.000000     0.189645    -0.000000    Biso  1.000000 O
O24         1.0    -0.000000     0.810355     0.000000    Biso  1.000000 O
```

Rb_6IrO_6

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
data_VESTA_phase_1

_chemical_name_common                  'Rb24 Ir4 O24                          '
_cell_length_a                         10.766218
_cell_length_b                         10.766218
_cell_length_c                         10.766218
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           1247.928004
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Rb1        1.0     0.000000     0.750000     0.750000    Biso  1.000000 Rb
   Rb2        1.0     0.250000    -0.000000     0.750000    Biso  1.000000 Rb
   Rb3        1.0     0.000000     0.250000     0.750000    Biso  1.000000 Rb
   Rb4        1.0     0.750000    -0.000000     0.750000    Biso  1.000000 Rb
   Rb5        1.0     0.250000     0.750000    -0.000000    Biso  1.000000 Rb
   Rb6        1.0     0.250000     0.250000    -0.000000    Biso  1.000000 Rb
   Rb7        1.0     0.000000     0.250000     0.250000    Biso  1.000000 Rb
   Rb8        1.0     0.250000     0.500000     0.250000    Biso  1.000000 Rb
   Rb9        1.0     0.000000     0.750000     0.250000    Biso  1.000000 Rb
   Rb10       1.0     0.750000     0.500000     0.250000    Biso  1.000000 Rb
   Rb11       1.0     0.250000     0.250000     0.500000    Biso  1.000000 Rb
   Rb12       1.0     0.250000     0.750000     0.500000    Biso  1.000000 Rb
   Rb13       1.0     0.500000     0.750000     0.250000    Biso  1.000000 Rb
```

Rb14	1.0	0.750000	-0.000000	0.250000	Biso	1.000000 Rb
Rb15	1.0	0.500000	0.250000	0.250000	Biso	1.000000 Rb
Rb16	1.0	0.250000	-0.000000	0.250000	Biso	1.000000 Rb
Rb17	1.0	0.750000	0.750000	0.500000	Biso	1.000000 Rb
Rb18	1.0	0.750000	0.250000	0.500000	Biso	1.000000 Rb
Rb19	1.0	0.500000	0.250000	0.750000	Biso	1.000000 Rb
Rb20	1.0	0.750000	0.500000	0.750000	Biso	1.000000 Rb
Rb21	1.0	0.500000	0.750000	0.750000	Biso	1.000000 Rb
Rb22	1.0	0.250000	0.500000	0.750000	Biso	1.000000 Rb
Rb23	1.0	0.750000	0.250000	-0.000000	Biso	1.000000 Rb
Rb24	1.0	0.750000	0.750000	-0.000000	Biso	1.000000 Rb
Ir1	1.0	0.000000	-0.000000	-0.000000	Biso	1.000000 Ir
Ir2	1.0	0.000000	0.500000	0.500000	Biso	1.000000 Ir
Ir3	1.0	0.500000	-0.000000	0.500000	Biso	1.000000 Ir
Ir4	1.0	0.500000	0.500000	-0.000000	Biso	1.000000 Ir
O1	1.0	0.500000	-0.000000	0.685370	Biso	1.000000 O
O2	1.0	0.000000	-0.000000	0.814630	Biso	1.000000 O
O3	1.0	0.185370	-0.000000	-0.000000	Biso	1.000000 O
O4	1.0	0.814630	-0.000000	-0.000000	Biso	1.000000 O
O5	1.0	0.500000	0.685370	-0.000000	Biso	1.000000 O
O6	1.0	0.500000	0.314630	-0.000000	Biso	1.000000 O
O7	1.0	0.500000	0.500000	0.185370	Biso	1.000000 O
O8	1.0	0.000000	0.500000	0.314630	Biso	1.000000 O
O9	1.0	0.185370	0.500000	0.500000	Biso	1.000000 O
O10	1.0	0.814630	0.500000	0.500000	Biso	1.000000 O
O11	1.0	0.500000	0.185370	0.500000	Biso	1.000000 O
O12	1.0	0.500000	0.814630	0.500000	Biso	1.000000 O
O13	1.0	0.000000	-0.000000	0.185370	Biso	1.000000 O
O14	1.0	0.500000	-0.000000	0.314630	Biso	1.000000 O
O15	1.0	0.685370	-0.000000	0.500000	Biso	1.000000 O
O16	1.0	0.314630	-0.000000	0.500000	Biso	1.000000 O
O17	1.0	0.000000	0.685370	0.500000	Biso	1.000000 O
O18	1.0	0.000000	0.314630	0.500000	Biso	1.000000 O
O19	1.0	0.000000	0.500000	0.685370	Biso	1.000000 O
O20	1.0	0.500000	0.500000	0.814630	Biso	1.000000 O
O21	1.0	0.685370	0.500000	-0.000000	Biso	1.000000 O
O22	1.0	0.314630	0.500000	-0.000000	Biso	1.000000 O
O23	1.0	0.000000	0.185370	-0.000000	Biso	1.000000 O
O24	1.0	0.000000	0.814630	-0.000000	Biso	1.000000 O