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Electronic Supplementary Material

Machine learning facilitated by microscopic features for discovery of novel magnetic double perovskites

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Table S1: Experimatal magnetic order, label used in classification model, experimental transition temperature ($T_{c\text{-}Exp}$), Curie-Weiss temperature (Θ_{Exp}) and frustrated factor(f_{Exp}) of AFM double perovskites.

Compound	Space group	Order	Label	$T_{c\text{-}Exp}$ K	Θ_{Exp} K	f_{Exp}
Ba_2CeIrO_6	$P2_1/n$	AFM	-1	-17 [1]	-177 [1]	10.4
Ca_2CoTeO_6	$P2_1/n$	AFM	-1	-10 [2]	-78 [2]	7.80
Ca_2CoWO_6	$P2_1/n$	AFM	-1	-33 [3]	-68 [3]	2.06
Ca_2FeSbO_6	$P2_1/n$	AFM	-1	-17 [4]	-90 [4]	5.23
Ca_2InOsO_6	$P2_1/n$	AFM	-1	-14 [5]	-77 [5]	5.50
Ca_2LaRuO_6	$P2_1/n$	AFM	-1	-11.5 [6]	-115 [6]	10.0
Ca_2LuRuO_6	$P2_1/n$	AFM	-1	-14 [6]	-162 [6]	11.5
Ca_2MnWO_6	$P2_1/n$	AFM	-1	-45 [7]	-61.8 [7]	1.37
Ca_2NiWO_6	$P2_1/n$	AFM	-1	-52.5 [8]	-75 [8]	1.42
In_2NiMnO_6	$P2_1/n$	AFM	-1	-26 [9]		
La_2CoRuO_6	$P2_1/n$	AFM	-1	-25 [10]	-87 [10]	3.48
La_2CoTiO_6	$P2_1/n$	AFM	-1	-14.8 [11]	-45 [12]	
La_2LiRuO_6	$P2_1/n$	AFM	-1	-30 [13]	-185 [14]	6.16
La_2MgIrO_6	$P2_1/n$	AFM	-1	-12 [15]	-24 [15]	2.00
La_2NaOsO_6	$P2_1/n$	AFM	-1	-12 [16]	-74 [16]	6.16
La_2NaRuO_6	$P2_1/n$	AFM	-1	-15 [16]	-67 [17]	4.46
La_2NiIrO_6	$P2_1/n$	AFM	-1	-110 [18]	-36 [19]	0.32
La_2NiRuO_6	$P2_1/n$	AFM	-1	-20 [20]	-90 [20]	4.50
La_2NiTiO_6	$P2_1/n$	AFM	-1	-23 [21, 22]	-60 [21, 22]	2.60
La_2ZnIrO_6	$P2_1/n$	Canted AFM[23]	-1	-7.5 [15, 24]	-3.1 [15]	0.41
Mn_2MnReO_6	$P2_1/n$	AFM[25]				
Sr_2CaIrO_6	$P2_1/n$	AFM	-1	-58 [26]	-363.4 [26]	6.26
Sr_2CeIrO_6	$P2_1/n$	AFM	-1	-21 [27]	-108 [28]	5.14
Sr_2CoTeO_6	$P2_1/n$	AFM	-1	-15 [2]	-146 [2]	9.73
Sr_2DyRuO_6	$P2_1/n$	AFM	-1	-21.3 [29]	-20 [30]	
Sr_2FeWO_6	$P2_1/n$	AFM	-1	-37 [31]	-21.3 [31]	0.93
Sr_2GdRuO_6	$P2_1/n$	AFM	-1	-33 [32]	-8 [33]	0.24
Sr_2LuRuO_6	$P2_1/n$	AFM	-1	-32 [33]	-353 [34]	11.0
Sr_2MnMoO_6	$P2_1/n$	AFM	-1	-15 [35]	-163 [36]	10.8
Sr_2MnUO_6	$P2_1/n$	AFM	-1	-21 [37]		
Sr_2MnWO_6	$P2_1/n$	AFM	-1	-13.7 [35]	-71.3 [38]	5.20
Sr_2NiIrO_6	$P2_1/n$	AFM	-1	-58 [39]	-81 [40]	1.39
Sr_2NiUO_6	$P2_1/n$	AFM	-1	-21 [37]		
Sr_2ScReO_6	$P2_1/n$	AFM	-1	-75 [41]	-450 [41]	6.00
Sr_2TmRuO_6	$P2_1/n$	AFM	-1	-36 [42]	-47 [33]	1.30
Sr_2YbRuO_6	$P2_1/n$	AFM	-1	-44 [42]	-225 [33]	5.11
Sr_2YIrO_6	$P2_1/n$	AFM	-1	-1.3 [43]	-2.8 [44]	2.15
Sr_2ZnIrO_6	$P2_1/n$	AFM[45]	-1			
Y_2CoMnO_6	$P2_1/n$	AFM[46]	-1		-80[47]	
Ba_2CaIrO_6	$Fm\overline{3}m$	AFM	-1	-55 [48]	-573[49]	10.4
Ba_2CaOsO_6	$Fm\overline{3}m$	AFM	-1	-50 [50, 22]	-156 [51]	3.12
Ba_2CaReO_6	$Fm\overline{3}m$	AFM	-1	-15.4 [51]	-41.5[52]	
Ba_2CoReO_6	$Fm\overline{3}m$	AFM	-1	-41 [53]	-35 [53]	2.69

Ba_2CoWO_6	$Fm\bar{3}m$	AFM	-1	-18 [3]	-75.2 [54]	4.17
Ba_2ErRuO_6	$Fm\bar{3}m$	AFM	-1	-40 [55]	-14.6 [55]	0.365
Ba_2LiOsO_6	$Fm\bar{3}m$	AFM	-1	-8 [56]	-40 [56]	5.00
Ba_2LuRuO_6	$Fm\bar{3}m$	AFM	-1	-35 [34]	-630 [34]	18.0
Ba_2MnWO_6	$Fm\bar{3}m$	AFM	-1	-9 [57]	-64.4 [57]	7.15
Ba_2MnMoO_6	$Fm\bar{3}m$	AFM	-1	-10 [58]	-94 [58]	
Ba_2NiWO_6	$Fm\bar{3}m$	AFM	-1	-48 [59]	-120 [59]	2.50
Ba_2PrIrO_6	$Fm\bar{3}m$	AFM	-1	-71 [60]	-43 [61]	0.60
Ba_2PrRuO_6	$Fm\bar{3}m$	AFM	-1	-117 [62]	-133 [62]	1.13
Ba_2YReO_6	$Fm\bar{3}m$	AFM[63]	-1		-616 [51]	
Ba_2YRuO_6	$Fm\bar{3}m$	AFM	-1	-36 [64]	-571 [64]	15.8
Sr_2ZrMnO_6	$Fm\bar{3}m$	AFM	-1	-50 [65]	-53.24 [65]	1.06
Ba_2CuOsO_6	$I4/m$	AFM	-1	-70 [66]	-13.3[66]	0.19
Ba_2CuWO_6	$I4/m$	Quasi-2D AFM	-1	-28 [67]	-180 [68]	6.42
Ba_2FeWO_6	$I4/m$	AFM	-1	-19 [69]		
Sr_2CoMoO_6	$I4/m$	AFM	-1	-37 [70]	-40 [35]	1.08
Sr_2CoOsO_6	$I4/m$	AFM	-1	-108 [71]	-51 [71]	0.47
Sr_2CoReO_6	$I4/m$	AFM	-1	-60 [72]	-140 [72]	2.33
Sr_2CoWO_6	$I4/m$	AFM	-1	-24 [3]	-57 [3]	2.37
Sr_2CuMoO_6	$I4/m$	AFM	-1	-28 [73]	-300 [73]	10.7
Sr_2CuOsO_6	$I4/m$	AFM	-1	-18 [74]	-40 [74]	2.22
Sr_2CuWO_6	$I4/m$	AFM	-1	-24 [73]	-230[75]	9.58
Sr_2MgOsO_6	$I4/m$	AFM	-1	-110 [22]	-347 [22]	3.15
$Sr_2NiMoO6$	$I4/m$	AFM	-1	-71.5 [76]	-260 [76]	3.63
Sr_2NiOsO_6	$I4/m$	AFM	-1	-50 [77]	27 [77]	0.54
Sr_2NiReO_6	$I4/m$	AFM	-1	-30 [72]		
Sr_2NiWO_6	$I4/m$	AFM	-1	-54 [78]	-175 [78]	3.24

Table S2: Experimatal magnetic behavior, label used in classification model and transition temperature ($T_{c\text{-}Exp}$) of FM double perovskites.

Compound	Space group	Order	Label K	$T_{c\text{-}Exp}$
Ca_2CoReO_6	$P2_1/n$	FM	1	130 [41]
Ca_2CrReO_6	$P2_1/n$	FM	1	360 [41]
Ca_2CrSbO_6	$P2_1/n$	FM	1	13 [79]
Ca_2FeMoO_6	$P2_1/n$	FiM	1	380 [80]
Ca_2FeOsO_6	$P2_1/n$	FiM	1	320 [81]
Ca_2FeReO_6	$P2_1/n$	FiM	1	540 [82]
Ca_2MnReO_6	$P2_1/n$	FM	1	110 [41]
La_2CoMnO_6	$P2_1/n$	FM	1	204 [83]
La_2NiMnO_6	$P2_1/n$	FM	1	280 [84]
Lu_2NiMnO_6	$P2_1/n$	FM	1	45 [85]
Sr_2FeUO_6	$P2_1/n$	FiM	1	150 [37]
Sr_2MnReO_6	$P2_1/n$	FiM	1	120 [41]
Tm_2NiMnO_6	$P2_1/n$	FM	1	
Y_2NiMnO_6	$P2_1/n$	FM	1	85 [86]
Ba_2FeReO_6	$Fm\overline{3}m$	FiM	1	317 [87]
Ba_2FeUO_6	$Fm\overline{3}m$	FiM	1	120 [88]
Ba_2MnReO_6	$Fm\overline{3}m$	FM	1	113 [89]
Ba_2NaOsO_6	$Fm\overline{3}m$	FM	1	6.8 [90]
Ba_2NiReO_6	$Fm\overline{3}m$	FM	1	32 [89]
Ba_2NiUO_6	$Fm\overline{3}m$	FM	1	25 [88]
Sr_2FeMoO_6	$I4/m$	FiM	1	400 [91]
Sr_2FeReO_6	$I4/m$	FiM	1	445 [92]

Table S3: ML predicted magnetic transition temperature ($T_{c\text{-}ML}$) and recent experimental reports ($T_{c\text{-}Exp}$) of 7 FM candidates.

Compound	Space group	$T_{c\text{-}ML}$ K	$T_{c\text{-}Exp}$ K
Bi_2NiMnO_6	$P2_1/n$	172	
Ca_2MgOsO_6	$P2_1/n$	52	-19 [22]
Sr_2CrSbO_6	$P2_1/n$	57	-12 [93]
Ba_2FeMoO_6	$Fm\overline{3}m$	209	345 [94]
Ba_2NaReO_6	$Fm\overline{3}m$	34	
Ca_2TiSiO_6	$Fm\overline{3}m$	34	
Ca_2TiMnO_6	$I4/m$	99	

Table S4: ML predicted magnetic transition temperature ($T_{c\text{-}ML}$), Curie-Weiss temperature (Θ_{ML}), frustration factor (f_{ML}) and recent experimental reports ($T_{c\text{-}Exp}$, Θ_{Exp}, f_{Exp}) of 45 AFM candidates.

Compound	Space group	$T_{c\text{-}ML}$ K	Θ_{ML} K	f_{ML}	$T_{c\text{-}Exp}$ K	Θ_{Exp} K	f_{Exp}
Ba_2LaRuO_6	$P2_1/n$	-30.7	-127.4	4.1			
Ca_2CaWO_6	$P2_1/n$	-28.6	-153.5	5.3			
Ca_2MgWO_6	$P2_1/n$	-28.7	-151.7	5.3			
Ca_2ScOsO_6	$P2_1/n$	-33.3	-201.9	6.0	-69 [95]	-341 [95]	
La_2CoPtO_6	$P2_1/n$	-34.7	-121.2	3.5	-28 [96]	-28 [96]	
La_2LiMoO_6	$P2_1/n$	-24.4	-121.3	4.9	-18 [97]	-59 [97]	
La_2LiReO_6	$P2_1/n$	-27.9	-172.0	6.1		-204 [98]	4 [99]
La_2MgPtO_6	$P2_1/n$	-33.3	-127.1	3.8			
La_2MgTiO_6	$P2_1/n$	-22.9	-107.1	4.6			
La_2MnVO_6	$P2_1/n$	-29.3	-70.4	2.4			
La_2NiPtO_6	$P2_1/n$	-36.9	-142.9	3.8			
Sr_2CaMoO_6	$P2_1/n$	-30.2	-179.1	5.9			
Sr_2CoReO_6	$P2_1/n$	-40.9	-75.4	1.8			
Sr_2CoWO_6	$P2_1/n$	-38.7	-75.6	1.9			
Sr_2MgIrO_6	$P2_1/n$	-33.1	-200.1	6.0	-74 [26]	-418 [26]	
Sr_2ScOsO_6	$P2_1/n$	-41.8	-273.4	6.5	-92 [100]	-677 [100]	
Y_2MgTiO_6	$P2_1/n$	-23.8	-96.1	4.0			
Ba_2CaMoO_6	$Fm\overline{3}m$	-41.8	-95.7	2.3			
Ba_2CdOsO_6	$Fm\overline{3}m$	-18.9	-134.9	7.1			
Ba_2CdReO_6	$Fm\overline{3}m$	-14.6	-75.8	5.1	-12 [101]	-15.3 [101]	
Ba_2EuReO_6	$Fm\overline{3}m$	-50.4	-572.7	11.3			
Ba_2LaReO_6	$Fm\overline{3}m$	-42.1	-521.6	12.4			
Ba_2LiReO_6	$Fm\overline{3}m$	-17.2	-70.0	4.0			
Ba_2MgOsO_6	$Fm\overline{3}m$	-43.1	-162.5	3.8	-53 [102]	-149 [102]	2 [102]
Ba_2MgWO_6	$Fm\overline{3}m$	-23.6	-87.3	3.7			
Ba_2LuReO_6	$Fm\overline{3}m$	-43.5	-485.2	11.1	-31 [103]	-678 [103]	
Ba_2ScRuO_6	$Fm\overline{3}m$-HP	-38.9	-287.3	7.4	-44 [104]	-651 [104]	
Ba_2SmReO_6	$Fm\overline{3}m$	-48.1	-533.1	11.0			
Ba_2TbReO_6	$Fm\overline{3}m$	-51.1	-503.6	7.4			
Ba_2YbReO_6	$Fm\overline{3}m$	-49.4	-525.9	10.6			
Ba_2YOsO_6	$Fm\overline{3}m$	-44.2	-213.2	4.8	-69 [105]	-700 [105]	
Ba_2ZnOsO_6	$Fm\overline{3}m$	-17.3	-156.4	9.0			
Ba_2ZnReO_6	$Fm\overline{3}m$	-14.1	-71.5	5.0	11 (FM) [106]	-66 [106]	
Ba_2ZnWO_6	$Fm\overline{3}m$	-25.2	-93.4	3.7			
Sr_2GdReO_6	$Fm\overline{3}m$	-50.7	-505.6	9.9			
Sr_2LiReO_6	$Fm\overline{3}m$	-22.8	-84.5	3.7			
Sr_2MgIrO_6	$Fm\overline{3}m$	-31.4	-341.0	10.8	-80 [107]		
Sr_2TmReO_6	$Fm\overline{3}m$	-47.8	-516.5	10.7			
Sr_2YbReO_6	$Fm\overline{3}m$	-47.3	-511.2	10.8			
Sr_2YReO_6	$Fm\overline{3}m$	-46.6	-491.0	10.5			
Sr_2ZnWO_6	$Fm\overline{3}m$	-22.5	-53.8	2.4			
Ba_2CaReO_6	$I4/m$	-37.5	-201.4	5.3			
Sr_2CoWO_6	$I4/m$	-36.7	-57	1.5			

Sr_2NiWO_6	$I4/m$	-44.1	-175	3.9
Sr_2ZnReO_6	$I4/m$	-38.7	-187.8	4.8

Resampled regression model of AFM/FM transition temperatures

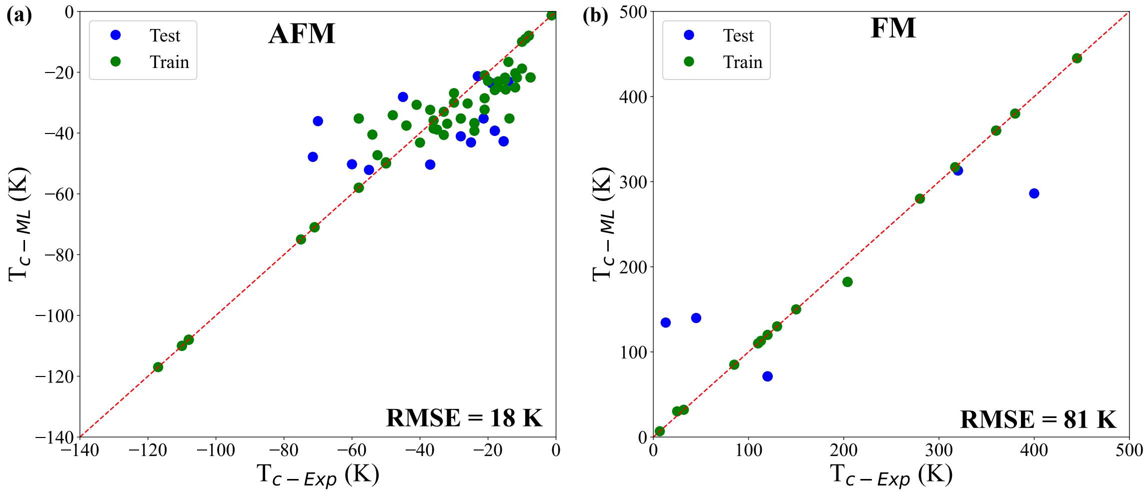

Fig. S1: Magnetic transition temperature T_c by the regression models with randomly doubled 11 and 2 (3 and 1) training (testing) samples for the (a) antiferromagnetic and (b) ferromagnetic materials in comparsion with the experimental value. The training and testing datasets are green and blue dots, respectively.

DFT+U+SOC calculations of cubic Ba_2LaReO_6

We performed DFT+U+SOC calculations on two magnetic configurations: FM (Fig. S2a) and AFM-I (Fig. S2b) type. AFM-I case is the experimental most observed pattern for cubic double perovskites, where in-plane NN are FM, while out-of-plane NN are AFM.

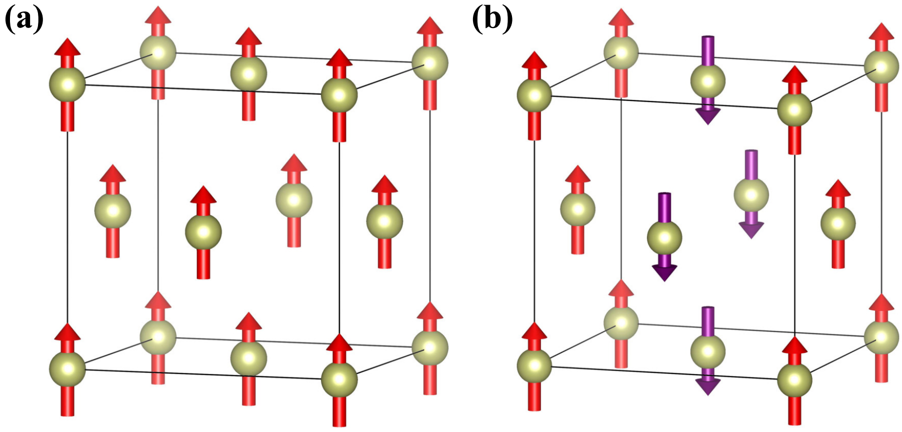

Fig. S2: (a) FM and (b) AFM-I configurations of cubic Ba_2LaReO_6.

DFT+U+SOC calculations of monoclinic Ba_2LaRuO_6

Low-symmetry monoclinc structure needs more magnetic configurations. Therefore, DFT+U+SOC calculations of 2*2*1 supercell on one FM and six AFM configurations are performed. $J_{d'}^{B'\text{-}B'}$ is considered the same as $J_d^{B'\text{-}B'}$ for simplication, leaving 4 $J_a^{B'\text{-}B'}S$, 4 $J_b^{B'\text{-}B'}$ and 32 $J_d^{B'\text{-}B'}$ for each configuration. The total energies by Heisenberg Hamiltonian can be written as

$E_{FM} = E_0 + 4\ J_a^{B'\text{-}B'}S^2 + 4\ J_b^{B'\text{-}B'}S^2 + 32\ J_d^{B'\text{-}B'}S^2$

$E_{AFM\text{-}I} = E_0 + 4\ J_a^{B'\text{-}B'}S^2 + 4\ J_b^{B'\text{-}B'}S^2 - 32\ J_d^{B'\text{-}B'}S^2$

$E_{AFM\text{-}II} = E_0 + 4\ J_a^{B'\text{-}B'}S^2 - 4\ J_b^{B'\text{-}B'}S^2$

$E_{AFM\text{-}III} = E_0 + 4\ J_a^{B'\text{-}B'}S^2 - 4\ J_b^{B'\text{-}B'}S^2$

$E_{AFM\text{-}IV} = E_0 - 4\ J_a^{B'\text{-}B'}S^2 + 4\ J_b^{B'\text{-}B'}S^2$

$E_{AFM\text{-}V} = E_0 - 4\ J_a^{B'\text{-}B'}S^2 - 4\ J_b^{B'\text{-}B'}S^2$

$E_{AFM\text{-}VI} = E_0 - 8\ J_d^{B'\text{-}B'}S^2$

where S is 3/2 for Ru. In Table S3, the DFT+U+SOC calculated total energies are compared with the counterpart Heisenberg Hamiltonians. The residual sum of squares is about 0.0044 meV. The $J_a^{B'\text{-}B'}$, $J_b^{B'\text{-}B'}$, $J_d^{B'\text{-}B'}$ and $J_{d'}^{B'\text{-}B'}$ are 2.12, 1.72, 0.93 and 0.93 meV (24.6, 20, 10.8 and 10.8 K).

Table S5: The total energy differences (meV/f.u.) of six AFM congurations compared to that of FM configuration.

Configuration	DFT+U+SOC	Heisenberg model
AFM-I	-135.21	-135.25
AFM-II	-102.44	-98.62
AFM-III	-102.44	-98.62
AFM-IV	-111.60	-105.88
AFM-V	-134.92	-136.87
AFM-VI	-121.23	-119.15

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