Supplemental material: Benchmark for *ab initio* prediction of magnetic structures based on cluster multipole theory

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I. DETAILS OF VASP SETUP

The flags in the `INCAR` file are set a follows:

- First try: `ENCUT`= 520, `EDIFF` = 10^{-8}, `ISMEAR` = 0, `SIGMA` = 0.02, `NELM` = 999, `LSORBIT` = True, `LNONCOLLINEAR` = True, `NPAR` = 4, `LORBIT` = 11, `LORBMOM` = True, `MAGMOM`= (*material dependent*)
- Second try: `IALGO` = 58, `AMIX_MAG` = 0.1, `BMIX_MAG` = 0.0001 , `ENCUT`= 520, `EDIFF` = 10^{-8}, `ISMEAR` = 0, `SIGMA` = 0.02, `NELM` = 999, `LSORBIT` = True, `LNONCOLLINEAR` = True, `NPAR` = 4, `LORBIT` = 11, `LORBMOM` = True, `MAGMOM`= (*material dependent*)
- Third try: `IALGO` = 58, `ENCUT`= 520, `EDIFF` = 10^{-6}, `ISMEAR` = 0, `SIGMA` = 0.02, `NELM` = 999, `LSORBIT` = True, `LNONCOLLINEAR` = True, `NPAR` = 4, `LORBIT` = 11, `LORBMOM` = True, `MAGMOM`= (*material dependent*)
- Fourth try: `IALGO` = 58, `AMIX_MAG` = 0.1, `BMIX_MAG` = 0.0001, `ENCUT`= 520, `EDIFF` = 10^{-6}, `ISMEAR` = 0, `SIGMA` = 0.02, `NELM` = 999, `LSORBIT` = True, `LNONCOLLINEAR` = True, `NPAR` = 4, `LORBIT` = 11, `LORBMOM` = True, `MAGMOM`= (*material dependent*)

Finally, in the rare cases that none of the above converge we chose the most stable setting by visual inspection of the `OSZICAR` file and reduced `EDIFF` as needed. We note that there has been no material, where this procedure failed to find a converged magnetic LSDA result with `EDIFF` $\leq 10^{-5}$.

II. EXPERIMENTAL DATA

Table 1 contains a list of MAGNDATA [1] entries used in this study. Each `0.xxx.mcif` label is linked to its web-entry [2] and the corresponding experimental reference. The purpose of Table 1 is to allow quick access to the experimental data. Furthermore, the inequivalent magnetic sites that constitute magnetic clusters are listed as well. For each cluster, the experimental on-site magnetic moment μ_{exp}, the LSDA+CMP on-site magnetic moment μ_{th} and the individual contribution from spin and orbital angular momentum in LSDA+CMP μ_s and μ_l are presented. The number of degrees of freedom, that is directly related to the number of magnetic configurations in the CMP basis, is given, as well as the number of active CMPs in the experimental magnetic configuration.

Note that some entries either lack μ_{exp} or the number of active CMPs. This is because following the experimental references we could not validate some of the information due to various reasons. Some examples, where μ_{exp} could not be confirmed, include among others: `0.110.mcif` Cr_2O_3—here, the order was determined using second harmonic generation—`0.113.mcif` $NiCO_3$, `0.114.mcif` $MnCO_3$—here, the magnetic moment was given an arbitrary value. On the other hand, there are entries, where the exact magnetic order could not be confirmed. For instance, `0.154.mcif` $Er_2Ru_2O_7$, where MAGNDATA commented that not all possible alternative models seem to have been checked, or `0.155.mcif` $CaMnGe_2O_6$, where there is some controversy around the proposed magnetic order [3, 4].

Table 1: Experimental data.

`0.1.mcif` $LaMnO_3$ Ref. [5]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.87	3.51	3.53	0.01	2	12
`0.3.mcif` $LiCa_3OsO_6$ Ref. [6]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
O	0.0	0.10	0.09	0.01	0	24
Os	2.2	1.59	1.68	0.09	1	6
`0.4.mcif` Cr_2NiO_4 Ref. [7]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Cr	1.40	2.67	2.69	0.02	2	12
Ni	1.64	1.42	1.25	0.17	2	6
`0.5.mcif` Cr_2S_3 Ref. [8]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Cr	1.19	2.64	2.66	0.02	2	3
Cr	1.19	2.63	2.65	0.01	2	3
Cr	1.19	2.64	2.66	0.02	2	6
`0.6.mcif` $YMnO_3$ Ref. [9]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	2.90	3.45	3.47	0.02	2	18
`0.7.mcif` $ScMnO_3$ Ref. [9]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.03	3.37	3.39	0.02	2	18
`0.9.mcif` GdB_4 Ref. [10]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Gd	7.14	6.91	6.83	0.07	1	12
`0.10.mcif` $DyFeO_3$ Ref. [11]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Dy	1.0	− − −	− − −	− − −	0	24
Fe	1.04	− − −	− − −	− − −	0	24
`0.12.mcif` $U_3(Al_3Ru)_4$ Ref. [12]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
U	2.50	1.09	1.50	2.59	5	18
`0.13.mcif` Ca_3MnCoO_6 Ref. [13]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	0.66	0.02	0.02	0.0	1	6
Mn	1.93	2.49	2.47	0.01	1	6
`0.15.mcif` MnF_2 Ref. [14]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.6	4.53	4.53	0.00	1	6
`0.16.mcif` $EuTiO_3$ Ref. [15]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Eu	6.92	6.29	6.63	0.33	2	6
`0.17.mcif` $FePO_4$ Ref. [16]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.15	3.98	3.96	0.01	3	12
O	0.0	0.13	0.13	0.00	0	12
O	0.0	0.12	0.12	0.0	0	12

`0.18.mcif` $Ba(MnAs)_2$ Ref. [17]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.88	3.63	3.61	0.01	1	6

`0.19.mcif` $TiMnO_3$ Ref. [18]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.55	4.34	4.34	0.00	1	6

`0.20.mcif` $MnTe_2$ Ref. [19]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.27	4.07	4.03	0.03	1	12

`0.21.mcif` $NiPbO_3$ Ref. [20]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ni	1.69	− − −	− − −	− − −	0	12

`0.22.mcif` DyB_4 Ref. [21]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Dy	9.8	8.45	4.65	3.79	1	12

`0.23.mcif` $Ca_3Mn_2O_7$ Ref. [22]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	2.67	2.54	2.56	0.02	1	12

`0.24.mcif` $LiMnPO_4$ Ref. [23]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.9	4.49	4.49	0.0	2	12

`0.25.mcif` $NaOsO_3$ Ref. [24]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Os	1.0	0.87	0.93	0.06	2	12

`0.26.mcif` TmAgGe Ref. [25]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Tm	6.44	− − −	− − −	− − −	0	24

`0.27.mcif` $Y(Fe_2Ge)_2$ Ref. [26]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	0.63	1.98	1.92	0.05	2	12
Fe	0.63	1.96	1.90	0.06	2	12

`0.28.mcif` $LiFe(SiO_3)_2$ Ref. [27]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.67	4.07	4.05	0.01	3	12
O	0.0	0.15	0.15	0.0	0	12
O	0.0	0.14	0.14	0.0	0	12
O	0.0	0.14	0.14	0.00	0	12
O	0.0	0.14	0.13	0.00	0	12

`0.30.mcif` $YbMnO_3$ Ref. [28]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Yb	0.0	1.15	0.36	0.79	0	12
Mn	3.25	3.30	3.32	0.01	2	18

`0.36.mcif` NiF_2 Ref. [29]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ni	2.00	1.76	1.57	0.18	2	6

`0.37.mcif` $U_3Al_2Si_3$ Ref. [30]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
U	0.16	0.18	1.52	1.70	1	3
U	0.16	0.16	1.49	1.64	1	3
U	1.29	0.44	1.76	2.20	4	12
`0.39.mcif` $NaNd_2RuO_6$ Ref. [31]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Nd	2.24	0.82	2.75	3.51	3	12
Ru	1.61	1.53	1.46	0.07	2	6
`0.43.mcif` $HoMnO_3$ Ref. [32]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ho	4.17	9.35	3.73	5.62	1	6
Ho	1.31	9.32	3.75	5.57	1	12
Mn	3.31	3.47	3.49	0.02	2	18
`0.45.mcif` La_2NiO_4 Ref. [33]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ni	1.68	1.28	1.15	0.12	2	12
`0.50.mcif` $TiMnO_3$ Ref. [34]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.9	4.34	4.34	0.00	1	6
`0.56.mcif` $Ba_2CoGe_2O_7$ Ref. [35]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	2.89	2.74	2.52	0.21	2	6
`0.58.mcif` Al_2CoO_4 Ref. [36]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	1.9	2.68	2.50	0.18	1	6
`0.64.mcif` MnV_2O_4 Ref. [37]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.2	4.21	4.20	0.00	1	6
V	1.29	1.63	1.67	0.04	3	12
`0.66.mcif` Fe_2O_3 Ref. [38]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.22	3.58	3.56	0.02	2	12
`0.72.mcif` $CaMnBi_2$ Ref. [39]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.73	3.95	3.86	0.09	1	6
`0.73.mcif` $SrMnBi_2$ Ref. [39]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.75	4.01	3.91	0.09	1	6
`0.74.mcif` Mn_3CuN Ref. [40]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	2.47	2.91	2.90	0.01	– – –	– – –
`0.76.mcif` Cr_2TeO_6 Ref. [41]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Cr	2.45	2.64	2.68	0.03	1	12
`0.77.mcif` $Tb_2Ti_2O_7$ Ref. [42]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Tb	– – –	– – –	– – –	– – –	7	12

`0.78.mcif` $Ni(NO_3)_2$ Ref. [43]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Ni	1.33	− − −	− − −	− − −	0	24
Ni	1.33	− − −	− − −	− − −	0	24
`0.79.mcif` $CaIrO_3$ Ref. [44]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Ir	− − −	− − −	− − −	− − −	1	6
`0.80.mcif` U_2InPd_2 Ref. [45]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
U	1.40	1.10	1.60	2.70	1	12
`0.81.mcif` U_2SnPd_2 Ref. [45]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
U	1.89	1.06	1.66	2.73	1	12
`0.83.mcif` $LiFeP_2O_7$ Ref. [16]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.62	4.09	4.07	0.01	2	6
O	0.0	0.10	0.10	0.00	0	6
`0.88.mcif` $LiNiPO_4$ Ref. [46]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Ni	2.22	1.72	1.53	0.19	2	12
`0.89.mcif` $Ba(MnBi)_2$ Ref. [47]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.83	3.97	3.88	0.09	1	6
`0.95.mcif` $LiFePO_4$ Ref. [16]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.19	3.72	3.55	0.17	1	12
`0.96.mcif` $CoSO_4$ Ref. [48]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Co	3.21	2.82	2.59	0.23	3	12
`0.97.mcif` $Fe(SbO_2)_2$ Ref. [49]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Fe	3.68	3.70	3.55	0.14	3	12
`0.101.mcif` Mn_2GeO_4 Ref. [50]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.02	4.43	4.43	0.0	2	12
Mn	4.5	4.44	4.44	0.0	1	12
`0.105.mcif` $ErVO_3$ Ref. [51]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Er	8.2	6.89	2.41	4.47	1	12
V	1.47	0.07	0.08	0.03	2	12
`0.106.mcif` $DyVO_3$ Ref. [51]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Dy	7.76	8.43	4.65	3.77	2	12
V	1.45	1.68	1.70	0.03	2	12
`0.107.mcif` $Ho_2Ge_2O_7$ Ref. [52]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Ho	9.05	9.12	3.75	5.38	3	24

`0.109.mcif` Mn_3Pt Ref. [53]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	2.93	3.12	3.09	0.02	3	9
`0.110.mcif` Cr_2O_3 Ref. [54]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Cr	− − −	− − −	− − −	− − −	1	12
`0.111.mcif` $Nb_2Co_4O_9$ Ref. [55]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	3.0	2.62	2.43	0.19	1	12
Co	3.0	2.77	2.38	0.38	1	12
`0.112.mcif` $FeBO_3$ Ref. [56]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.7	3.91	3.89	0.02	1	6
`0.113.mcif` $NiCO_3$ Ref. [57]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ni	− − −	− − −	− − −	− − −	1	6
`0.114.mcif` $CoCO_3$ Ref. [58]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	− − −	− − −	− − −	− − −	1	6
`0.115.mcif` $MnCO_3$ Ref. [59]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	− − −	− − −	− − −	− − −	1	6
`0.116.mcif` $FeCO_3$ Ref. [60]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	− − −	− − −	− − −	− − −	1	6
`0.117.mcif` $LuFeO_3$ Ref. [61]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	2.90	3.64	3.61	0.05	2	18
O	0.0	0.12	0.12	0.00	0	18
`0.118.mcif` $Ba_5Co_5ClO_{13}$ Ref. [62]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	0.61	0.69	0.63	0.05	1	12
Co	2.21	2.67	2.59	0.08	1	12
Co	0.35	0.23	0.19	0.04	1	6
O	0.0	0.26	0.26	0.00	0	36
`0.119.mcif` $CoSe_2O_5$ Ref. [63]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	3.20	2.82	2.55	0.27	2	12
`0.121.mcif` $Li_2Co(SO_4)_2$ Ref. [64]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	3.33	2.90	2.62	0.28	3	6
`0.122.mcif` $Li_2Mn(SO_4)_2$ Ref. [64]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.58	4.52	4.52	0.0	3	6
`0.125.mcif` $MnGeO_3$ Ref. [65]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ge	0.0	0.10	0.10	0.00	0	6
Mn	4.6	3.65	3.66	0.00	1	6

`0.126.mcif` $NpCo_2$ Ref. [66]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Np	0.5	0.04	1.35	1.31	1	6
`0.128.mcif` $FeSO_4F$ Ref. [67]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.32	4.06	4.04	0.01	1	6
`0.130.mcif` $Cu_3Mo_2O_9$ Ref. [68]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Cu	0.08	− − −	− − −	− − −	2	12
Cu	0.62	0.62	0.52	0.09	2	12
Cu	0.62	0.55	0.51	0.03	2	12
O	0.0	0.22	0.22	0.00	0	12
`0.131.mcif` $Mn(C_2N_3)_2$ Ref. [69]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Mn	5.01	4.41	4.42	0.00	1	6
`0.132.mcif` $Fe(C_2N_3)_2$ Ref. [69]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.11	3.73	3.51	0.22	2	6
`0.133.mcif` $Ni_3B_7ClO_{13}$ Ref. [70]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Ni	1.65	1.79	1.56	0.23	1	12
Ni	0.79	1.70	1.47	0.23	1	12
Ni	0.79	0.16	0.11	0.07	1	12
`0.137.mcif` $V_2Cu_2O_7$ Ref. [71]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Cu	0.93	0.54	0.48	0.06	2	12
`0.138.mcif` $CrBiO_3$ Ref. [72]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Cr	2.04	2.63	2.67	0.04	1	6
Cr	2.04	2.64	2.68	0.04	1	6
`0.140.mcif` $Lu(Fe_2Ge)_2$ Ref. [73]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Fe	0.44	1.93	1.86	0.06	2	12
Fe	0.44	1.79	1.73	0.05	2	12
`0.141.mcif` $TbGe_2$ Ref. [74]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Tb	7.55	7.73	5.74	1.99	1	6
Tb	9.45	7.73	5.81	1.92	1	6
`0.142.mcif` Fe_2TeO_6 Ref. [75]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.19	3.82	3.79	0.02	1	12
`0.143.mcif` Cr_2TeO_6 Ref. [75]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Cr	2.45	2.64	2.68	0.03	1	12
`0.146.mcif` $EuZrO_3$ Ref. [76]						
cluster	$\mu_{\rm exp}$	$\mu_{\rm th}$	μ_s	μ_l	active CMP	dgr. of freedom
Eu	7.3	6.67	6.75	0.08	2	12

`0.148.mcif` $LiLa_2RuO_6$ Ref. [77]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ru	2.20	1.82	1.84	0.01	2	6
O	0.0	0.12	0.11	0.00	0	12
O	0.0	0.11	0.11	0.00	0	12
O	0.0	0.10	0.10	0.00	0	12

`0.149.mcif` $Nd_3(Al_3Ru)_4$ Ref. [78]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Nd	2.09	0.19	3.22	3.41	2	18
Ru	0.0	0.13	0.11	0.01	0	18

`0.150.mcif` NiS_2 Ref. [79]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ni	0.98	0.47	0.44	0.03	1	12

`0.154.mcif` $Er_2Ru_2O_7$ Ref. [80]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Er	4.5	7.56	2.66	4.89	− − −	− − −
Ru	2.0	1.36	1.23	0.12	− − −	− − −

`0.155.mcif` $CaMn(GeO_3)_2$ Ref. [4]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.18	4.43	4.43	0.0	− − −	− − −

`0.157.mcif` $Yb_2Sn_2O_7$ Ref. [81]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
O	0.0	0.09	0.12	0.02	0	6
Yb	1.04	1.54	0.53	1.01	2	12

`0.158.mcif` $Yb_2Ti_2O_7$ Ref. [82]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Yb	0.89	1.54	0.53	1.00	2	12

`0.159.mcif` $DyCoO_3$ Ref. [83]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Dy	9.08	8.83	4.73	4.12	2	12

`0.160.mcif` $TbCoO_3$ Ref. [83]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Tb	8.26	7.69	5.74	1.95	2	12
Co	0.0	0.15	0.14	0.00	0	12

`0.163.mcif` $MnPS_3$ Ref. [84]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.43	4.25	4.25	0.00	2	6

`0.164.mcif` Y_2MnCoO_6 Ref. [85]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	− − −	− − −	− − −	− − −	3	6
Co	− − −	− − −	− − −	− − −	3	6

`0.165.mcif` $SrMnVHO_5$ Ref. [86]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.31	4.34	4.34	0.00	3	6
Mn	3.31	4.34	4.34	0.00	3	6

`0.167.mcif` $Nd_3Mg_2Sb_3O_{14}$ Ref. [87]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Nd	1.78	0.73	2.96	3.69	4	9

`0.168.mcif` $Fe_2H_4NF_6$ Ref. [88]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.12	3.93	3.81	0.12	3	12
Fe	3.12	4.09	3.92	0.16	1	12
`0.169.mcif` U_3As_4 Ref. [89]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
U	1.90	0.66	1.69	2.36	6	18
`0.170.mcif` U_3P_4 Ref. [89]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
U	1.47	0.43	1.61	2.04	6	18
`0.171.mcif` $DyScO_3$ Ref. [90]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Dy	9.46	8.88	4.77	4.12	2	12
`0.173.mcif` $Pr_3(Al_3Ru)_4$ Ref. [91]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Pr	− − −	− − −	− − −	− − −	2	18
`0.177.mcif` Mn_3GaN Ref. [92]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	1.17	2.59	2.57	0.01	3	9
`0.178.mcif` CoF_2 Ref. [93]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	2.6	2.91	2.62	0.29	1	6
`0.180.mcif` $MnPSe_3$ Ref. [94]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.74	4.22	4.20	0.01	1	6
`0.187.mcif` CeMnAsO Ref. [95]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ce	0.7	0.41	0.60	1.01	1	6
Mn	3.3	3.53	3.48	0.05	1	6
`0.189.mcif` $CeMn_2(GeO_3)_4$ Ref. [96]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.61	4.41	4.41	0.00	2	12
`0.191.mcif` $BaCuF_4$ Ref. [97]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Cu	0.83	− − −	− − −	− − −	0	6
`0.192.mcif` $RbFe_2F_6$ Ref. [98]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	3.99	4.06	3.93	0.12	1	12
Fe	4.29	3.93	3.84	0.10	3	12
`0.193.mcif` $LiCoPO_4$ Ref. [99]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	− − −	− − −	− − −	− − −	1	12
`0.194.mcif` $U(SiPt)_2$ Ref. [100]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
U	1.67	0.86	1.66	2.52	1	6

`0.198.mcif` $GdVO_4$ Ref. [101]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Gd	7.0	6.87	6.83	0.03	1	6

`0.199.mcif` Mn_3Sn Ref. [102]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	2.99	3.18	3.15	0.03	3	18

`0.203.mcif` Mn_3Ge Ref. [103]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	2.99	2.74	2.71	0.02	− − −	− − −

`0.204.mcif` Ca_2MnReO_6 Ref. [104]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.33	4.17	4.14	0.05	3	6
Re	0.21	0.20	0.46	0.25	2	6

`0.211.mcif` Ca_2MnO_4 Ref. [105]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	2.4	2.54	2.56	0.02	1	12

`0.212.mcif` $Sr_2Mn_3(AsO)_2$ Ref. [106]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.4	3.55	3.53	0.01	1	6

`0.215.mcif` $BaNi_2(PO_4)_2$ Ref. [107]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ni	2.00	1.72	1.55	0.17	2	6

`0.219.mcif` Co_2SiO_4 Ref. [108]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	3.87	2.59	2.40	0.18	3	12
Co	3.35	2.76	2.54	0.22	1	12
O	0.0	0.12	0.12	0.0	0	12

`0.220.mcif` Mn_2SiO_4 Ref. [109]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.84	4.44	4.44	0.0	3	12
Mn	4.67	4.45	4.45	0.0	2	12

`0.221.mcif` Fe_2SiO_4 Ref. [110]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	4.44	3.57	3.46	0.11	3	12
Fe	4.4	3.73	3.59	0.14	1	12
O	0.0	0.10	0.10	0.0	0	12

`0.222.mcif` MnCuAs Ref. [111]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	3.6	3.68	3.67	0.01	1	6

`0.228.mcif` $TbCo_2$ Ref. [112]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	1.19	1.28	1.16	0.12	1	9
Co	1.3	1.28	1.11	0.17	1	3
Tb	8.3	7.10	5.61	1.49	1	6

`0.229.mcif` $Ba_2MnSi_2O_7$ Ref. [113]

cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Mn	4.1	4.39	4.39	0.0	1	6

`0.230.mcif` $K_2CoP_2O_7$ Ref. [114]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Co	3.03	2.77	2.55	0.21	1	12
`0.235.mcif` $PrMn_2SbO_6$ Ref. [115]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Pr	2.2	1.63	1.93	3.56	1	12
Mn	5.1	4.43	4.43	0.0	1	6
Mn	5.1	4.44	4.44	0.00	1	6
Mn	5.1	4.41	4.40	0.00	1	12
`0.236.mcif` $Ca(Al_2Fe)_4$ Ref. [116]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Fe	0.71	3.26	3.11	0.15	2	12
`0.237.mcif` $Er_2Sn_2O_7$ Ref. [117]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Er	4.38	7.87	2.72	5.14	1	12
`0.238.mcif` $Er_2Pt_2O_7$ Ref. [118]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Er	4.80	7.73	2.70	5.03	1	12
`0.239.mcif` $LiCa_3RuO_6$ Ref. [119]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
O	0.0	0.10	0.1	0.00	0	24
Ru	2.8	1.78	1.80	0.02	1	6
`0.290.mcif` $CeCu_2$ Ref. [120]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Ce	0.33	0.04	0.31	0.36	1	6
`0.318.mcif` Tm_2MnCoO_6 Ref. [121]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Tm	2.17	5.03	1.62	3.40	3	12
Mn	2.82	3.35	3.38	0.03	2	6
Co	2.82	0.14	0.11	0.04	2	6
`0.408.mcif` PrSi Ref. [122]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Pr	2.80	0.11	2.23	2.15	2	12
`0.409.mcif` TmNi Ref. [123]						
cluster	μ_{exp}	μ_{th}	μ_s	μ_l	active CMP	dgr. of freedom
Tm	5.89	4.35	1.35	2.99	2	12

III. CMP BASIS, MAGNETIC DOMAINS AND LINEAR COMBINATIONS

Let us take $YMnO_3$ as an example material. The experimental details can be found in Table 1 or at the MAGNDATA entry `0.3.mcif`. Figure 1 shows 18 magnetic configurations that are in the CMP basis of $YMnO_3$. In other words, these 18 magnetic configurations span the space of possible magnetic configurations on the Mn-cluster in $YMnO_3$. The basis elements are ordered by their expansion order from 1 to 6. The Gram–Schmidt procedure leads to no basis element at order 5. The magnetic configurations within one box—additionally to having the same order—also share the same irreducible representation.

Following our proposed heuristic rule, we now construct equally weighted linear combinations of CMP basis elements that have the same order and same irreducible representation. As we have 6 pairs that fulfill this condition, this leads to additional 12 magnetic configurations. In each instance we consider the sum and the difference. The resulting configurations for the first order (red box in Figure 1) are shown in Figure 2. The upper (lower) row shows the

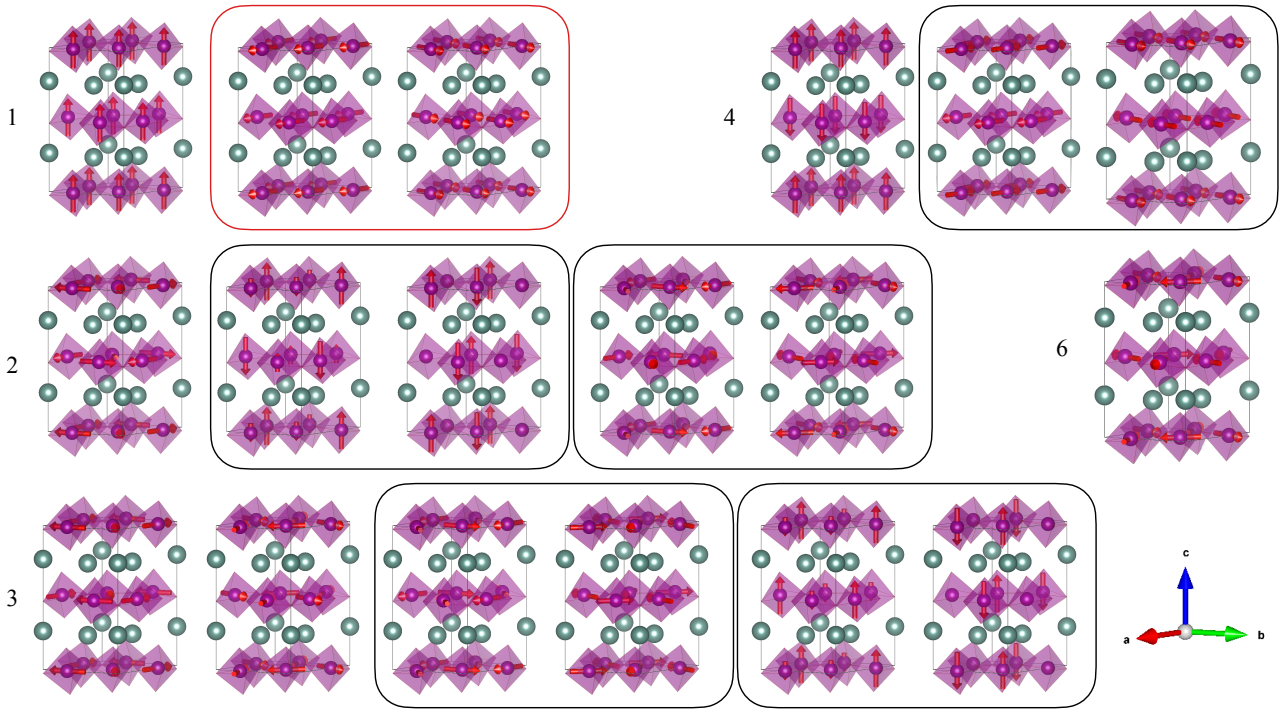

FIG. 1. Magnetic configurations in the CMP basis of $YMnO_3$.

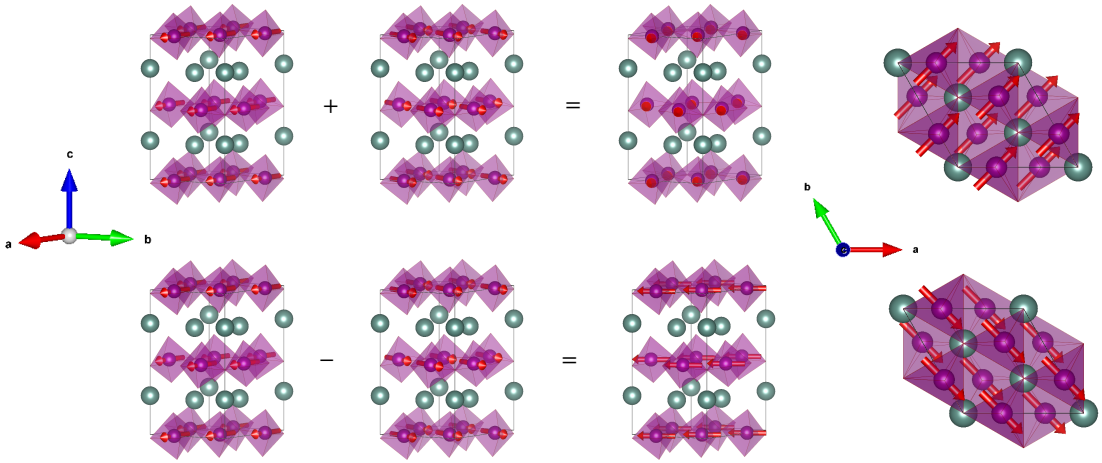

FIG. 2. Magnetic configurations corresponding to equally weighted linear combinations of CMPs with order 1 and same irreducible representation for $YMnO_3$.

addition (subtraction) of CMPs. The last column provides a top view of the resulting structure.

In the following we will see that the top and the bottom resulting configuration are actually redundant. This is because they are different domains of the same underlying magnetic configuration. Let us use this example to understand the notion of magnetic domains.

A magnetic domain corresponds to one possible realization of a magnetic configuration in a structure. Given the paramagnetic unit cell of a material, the set of all possible symmetry operations yields the space group (spg). In a magnetic material the spg of the paramagnetic system is often called parent spg, in contrast to the magnetic space group (mspg). The mspg contains all symmetry operations that consist of rotations, translations and time reversal, which leave the magnetic unit cell invariant. When we apply an spg operation, which is not element of the mspg, we

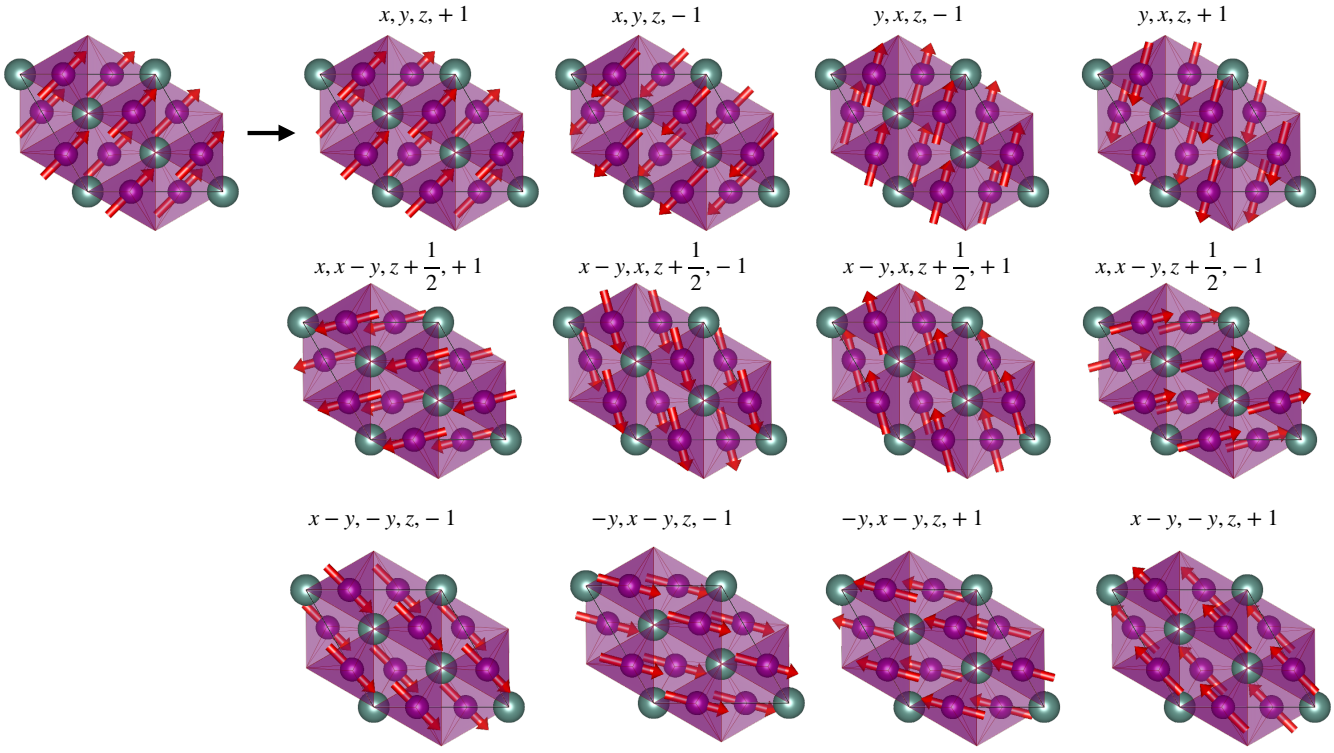

FIG. 3. Magnetic configurations corresponding to domains derived from the upper left configuration by application of the operation labeling the resulting magnetic configuration. The example material is $YMnO_3$.

obtain a different magnetic domain, but we explicitly do not change the magnetic structure.

Figure 3 presents all possible domains obtained for one magnetic configuration. The starting point is the magnetic configuration we obtained in the top row of Figure 2. Then, an operation which is element of the parent spg combined with both positive and negative time reversal symmetry is applied. The specific operation is written on top of each resulting configuration. Here, the operation is given in BNS setting as used by the Bilbao Crystallographic Server [124]. The careful reader may have noticed that the magnetic configuration obtained by application of $(x-y, -y, z, -1)$ exactly agrees with the magnetic configuration we obtained in the bottom row of Figure 2. In other words, these two candidates are redundant. We expect the LSDA result for both initial guesses to yield the exactly the same result up to numerical uncertainty. Therefore, the list of initial guesses should be screened for such redundant configurations within both the CMP basis and the additional linear combinations in order to avoid unnecessary computational cost.

IV. REPRODUCIBILITY

One of the core values of science as a whole is the reproducibility of a result. Especially in big data and high-throughput calculations, the meaning of reproducibility is different than in fields such as classical mechanics. Therefore, let us define reproducibility in the context of this study.

In Section III we have discussed that LSDA calculations starting from the same magnetic configuration are expected to yield the same converged result up to numerical uncertainty. Furthermore, we have introduced the notion of redundant candidates, that is two magnetic configurations which correspond to different magnetic domains of the same underlying magnetic structure. Neither the CMP basis nor the additional linear combinations that are introduced to create an exhaustive list of candidate magnetic configurations is generally free of such a redundancy. Without loss of exhaustiveness it is possible to avoid additional computational cost by excluding redundant candidates and only perform LSDA for unique candidates. In other words, it is sufficient to pick one realization of a magnetic structure and include it in the list of candidate magnetic configurations.

In this study, we did not filter the redundant candidates. This offers the opportunity to measure the reproducibility. We define reproducability as the probability to end up in the same local minimum under the condition that the initial candidates are equivalent up to their domain. Figure 4 visualizes how the reproducibility is computed.

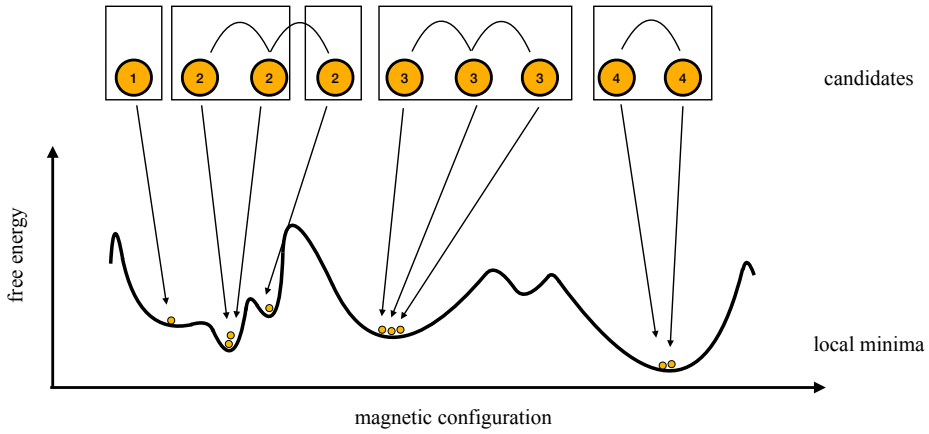

FIG. 4. Reproducibility.

For a given material, the list of candidates is generated, represented by yellow circles. Then each magnetic structure is given a unique number. Candidates with the same number hence correspond to different domains of the same magnetic structure. In the following this is referred to as candidate group. Independent LSDA calculations let each candidate fall into a local minimum in the LSDA total free energy landscape. For the converged magnetic configuration, again all possible domains are constructed. If two LSDA results are equivalent up to their domain, they are said to have fallen into the same local minimum. This is represented by boxes in Figure 4.

If we assume a bond between each candidate within a candidate group, then we expect these bonds to hold even after the LSDA calculation. In other words, each candidate group should map to one local minimum. This is the case for the magnetic structures labeled 3 and 4 in Figure 4. On the other hand, if candidates are at a very unstable initial position or many narrow local minima are present, then numerical uncertainty might indeed be enough impetus to converge to different magnetic structures. This is shown for the magnetic structures labeled 2 in Figure 4, where one of the bonds is severed. The reproducibility of one candidate group (g) is defined as

$$r_g = \frac{b_{\mathrm{us}}^{(g)}}{b_{\mathrm{tot}}^{(g)}}, \tag{1}$$

where b_{tot} is the total number of bonds and b_{us} is the number of unsevered bonds. Clearly, the magnetic structure labeled 1 in Figure 4 is not a candidate group of its own and is disregarded in the discussion about reproducibility. Finally, for the whole database we compute the expectation value of the reproducibility by summing over all entries and all candidate groups

$$\langle r \rangle = \sum_{\mathrm{entries}} \left(\sum_{g} r_g \right) \tag{2}$$

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