

## Supplementary Information

### Designing rare earth free permanent magnets: Insights from small Co clusters

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TABLE I: Spin moment ( $\mu_B$ ), point group (PG) symmetry, and MAE's (K) calculated by two different methods of  $\text{Co}_4\text{A}_2$  clusters. Clusters are identified by their relative energies (see Figure 2 in main text). Non-SC means charge density was kept constant while spin-orbit coupling is included. MAE SC means, charge density is varied to achieve self-consistency.

Relative energy	$M_s$	PG symmetry	MAE (Non SC)	MAE (SC)
<b><math>\text{Co}_4\text{C}_2</math></b>				
0.0	4	$C_s$	24.64	24.10
0.220	4	$C_s$	12.13	13.25
0.230	2	$C_s$	28.41	25.32
0.243	4	$C_2$	28.08	26.94
0.448	0	$C_s$	48.34	
<b><math>\text{Co}_4\text{Si}_2</math></b>				
0.0	6	$D_{2h}$	49.92	48.71
0.106	6	$D_{4h}$	35.12	34.55
0.439	4	$D_{4h}$	42.25	41.31
<b><math>\text{Co}_4\text{Ge}_2</math></b>				
0.0	6	$D_{4h}$	33.87	34.08
0.354	6	$C_s$	69.41	66.89
0.472	6	$C_{2v}$	62.58	61.84
<b><math>\text{Co}_4\text{N}_2</math></b>				
0.0	8	$C_s$	28.18	27.61
0.139	6	$C_{2v}$	48.62	
0.248	8	$C_s$	51.92	54.38
0.280	8	$C_s$	31.11	
0.404	8	$C_{2v}$	17.37	16.81
0.449	6	$C_{2v}$	60.67	56.51
<b><math>\text{Co}_4\text{P}_2</math></b>				
0.0	6	$C_{2v}$	35.12	31.84
0.041	8	$C_{2v}$	5.57	
0.082	6	$C_1$	26.13	24.96
0.110	6	$D_{4h}$	19.41	21.05
0.198	8	$C_s$	44.47	39.71
0.450	0	$C_{2v}$	17.50	16.87
0.459	4	$C_s$	29.14	30.97
<b><math>\text{Co}_4\text{As}_2</math></b>				
0.0	8	$D_{4h}$	50.14	41.80
0.034	8	$C_{2v}$	16.28	13.53
0.142	6	$C_{2v}$	39.32	
0.244	8	$C_s$	70.36	75.34
0.485	2	$C_s$	38.59	33.42