Electronic Supplementary Information for

Computational discovery of spin-polarized semimetals in spinel materials

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(Dated: April 27, 2022)

I. INFORMATION OF ALL SPINELS CONSIDERED

Table S1: The lattice constants (Con.) and magnetic moments (Mag.) of all spinels considered. The presence of spin-polarized (FSP) or semimetal (Semi.) states around the Fermi level is also discussed (Y: Yes, N: No).

		V				Co				Fe				Mn			
		Cons. (Å)	Mag. (μ_B)	FSP	Semi.	Cons. (Å)	Mag. (μ_B)	FSP	Semi.	Cons. (Å)	Mag. (μ_B)	FSP	Semi.	Cons. (Å)	Mag. (μ_B)	FSP	Semi.
AB_2O_4 oxide spinel	Ag	6.383	0.00	N	N	6.272	1.41	N	N	6.298	1.31	N	N	6.332	2.00	Y	N
	Al	5.875	6.00	Y	N	5.782	6.00	Y	N	5.814	8.00	N	N	5.858	10.00	Y	N
	Cd	6.405	0.00	N	N	6.370	10.00	Y	N	6.387	8.00	Y	N	6.384	6.00	Y	N
	Cu	5.977	2.00	Y	N	5.904	0.43	Y	N	5.924	4.00	Y	N	5.951	2.00	Y	N
	Ga	6.081	5.82	N	N	5.989	6.00	N	N	6.022	8.07	N	N	6.061	10.00	Y	N
	Ge	6.335	2.00	Y	N	6.198	4.88	Y	N	6.264	8.00	Y	N	6.282	8.67	N	N
	Hg	6.590	0.00	N	N	6.489	10.00	N	N	6.498	8.00	Y	N	6.508	6.00	N	N
	In	6.478	4.25	N	N	6.404	6.00	N	N	6.416	8.46	N	N	6.469	10.00	Y	N
	Ni	5.906	6.00	Y	N	5.819	2.00	N	N	5.848	4.00	Y	N	5.907	14.00	N	N
	Ti	6.077	5.81	N	N	5.945	2.78	N	N	6.042	5.64	N	N	6.103	7.40	N	N
	Y	6.588	6.00	Y	N	6.550	6.00	Y	N	6.560	8.00	N	N	6.514	10.00	Y	N
	Zn	6.033	2.00	Y	Y	5.945	10.00	Y	N	6.010	8.00	Y	N	6.008	6.00	Y	N
AB_2S_4 sulfide spinel	Ag	7.389	0.00	N	N	7.089	3.31	N	N	7.139	5.12	N	N	7.122	2.58	N	N
	Al	7.224	6.00	Y	N	6.996	6.00	Y	N	7.023	8.00	Y	N	7.132	10.00	Y	N
	Cd	7.643	2.00	Y	Y	7.206	4.39	N	N	7.263	8.100	N	N	7.366	6.00	Y	N
	Ga	7.326	5.66	Y	N	7.063	6.00	Y	N	7.088	8.00	Y	N	7.073	9.91	N	N
	Ge	7.485	3.46	N	N	7.083	4.48	N	N	7.017	7.37	N	N	7.257	8.27	N	N
	Hg	7.650	2.00	Y	Y	7.181	4.25	N	N	7.221	8.02	N	N	7.277	6.00	Y	N
	In	7.691	6.00	Y	N	7.270	6.00	Y	N	7.308	8.00	Y	N	7.431	10.00	Y	N
	Ni	6.925	0.00	N	N	6.623	0.00	N	N	6.630	3.39	N	N	6.683	4.77	N	N
	Ti	7.299	9.77	Y	N	7.018	2.88	N	N	7.053	8.63	N	N	7.174	10.00	N	N
	Y	7.848	6.00	Y	N	7.350	6.00	N	N	7.385	8.14	N	N	7.416	10.00	Y	N
	Zn	7.261	2.00	Y	N	6.923	4.19	N	N	7.049	8.00	N	N	7.143	6.00	Y	N

II. MAGNETIC CONFIGURATIONS AND ELASTIC CONSTANTS

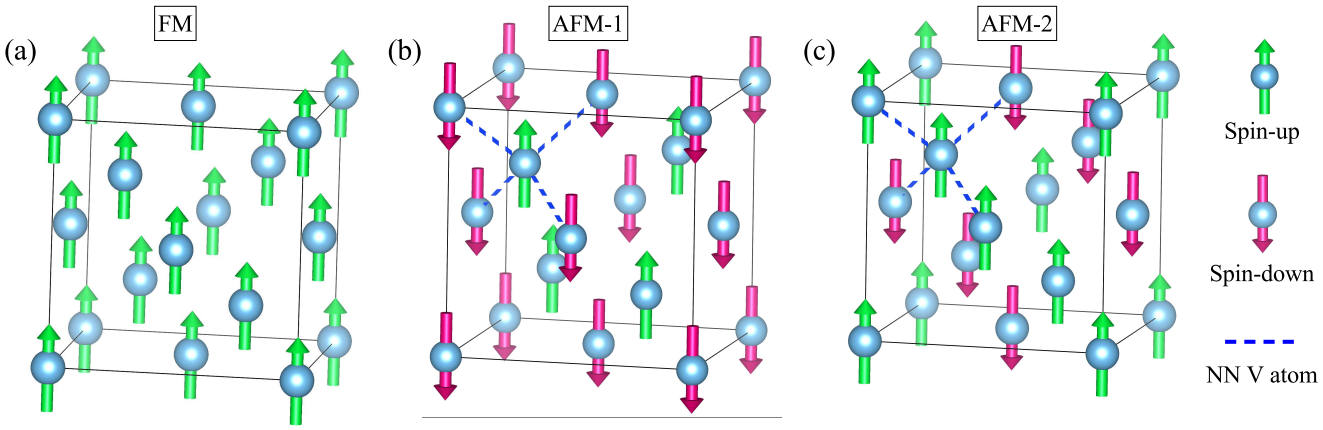

Figure S1: Illustrations of ferromagnetic and two types of antiferromagnetic configurations.

Table S2: Elastic constants C_{ij}(Gpa) of VZn_2O_4 and VCd_2S_4 at equilibrium lattice constant.

	C_{11}	C_{12}	C_{44}
VZn_2O_4	255.30	153.06	69.47
VCd_2S_4	97.96	54.81	22.31

III. ORBITAL RESOLVED BANDS AND LOCAL GAP DISTRIBUTION OF VCd_2S_4

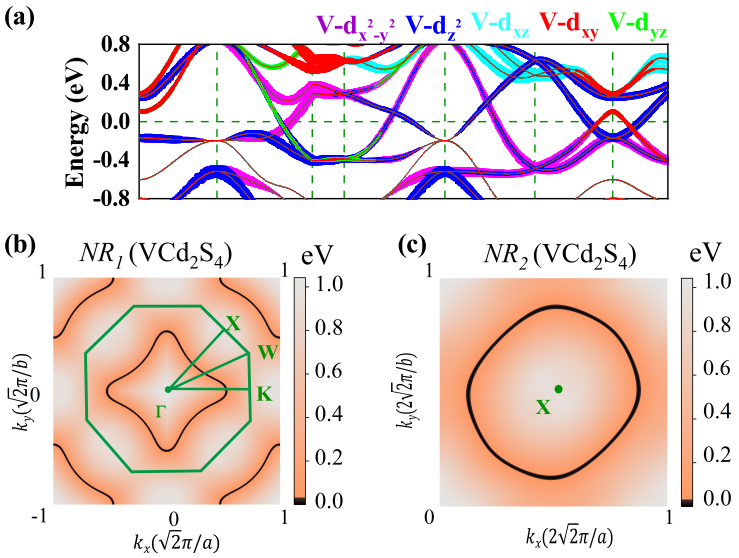

Figure S2: (a) Orbital resolved band structures of VCd_2S_4. (b) and (c) The local gaps between CBM and VBM of VCd_2S_4 in the k_z=0 and G-X-L planes, respectively.

IV. EIGENVALUES OF SYMMETRY OPERATIONS

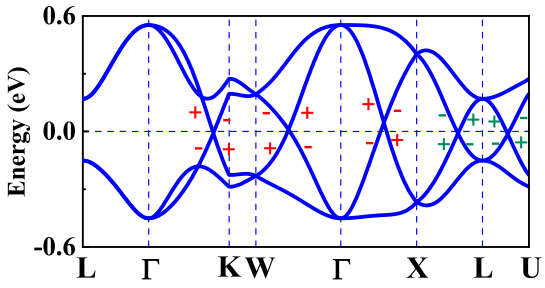

Figure S3: The enlarged band structures of VZn_2O_4 near the E_f and the opposite eigenvalues (± 1) under glide mirror operation G_z (red) and mirror operation $G_{\bar{1}01}$ (green).

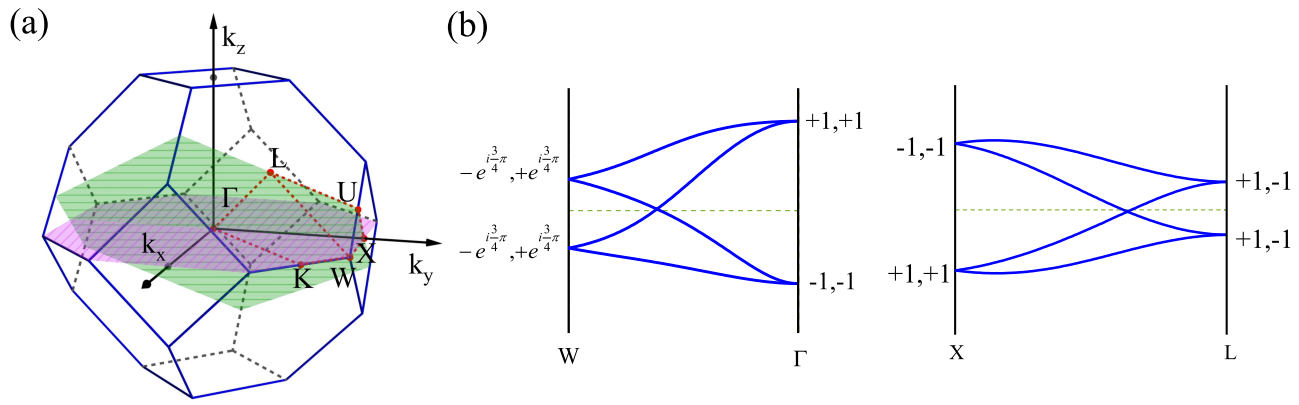

Figure S4: (a) Schematic diagram of invariant plane of G_z and $G_{\bar{1}01}$ in BZ (purple and green plane). (b) The four states' glide or mirror eigenvalues at four high symmetry points.

V. BERRY PHASE OF TB MODEL

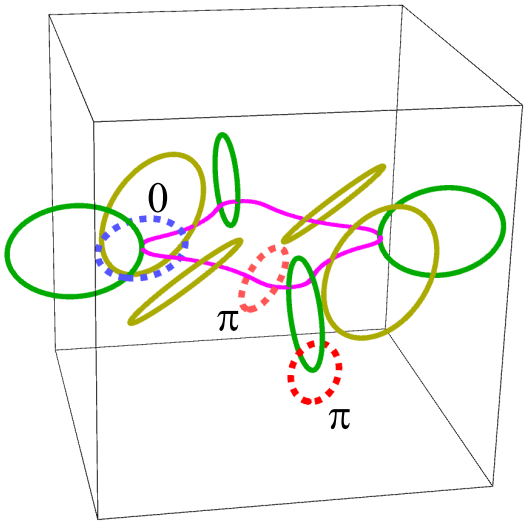

Figure S5: Schematic diagram of the values of Berry phase with different loops. The red and blue dotted loop, respectively, passes through one ring and two rings.

VI. ENERGY BAND STRUCTURES OF VZn_2O_4 WITH DIFFERENT HUBBARD U, DIFFERENT STRAINS AND SOC

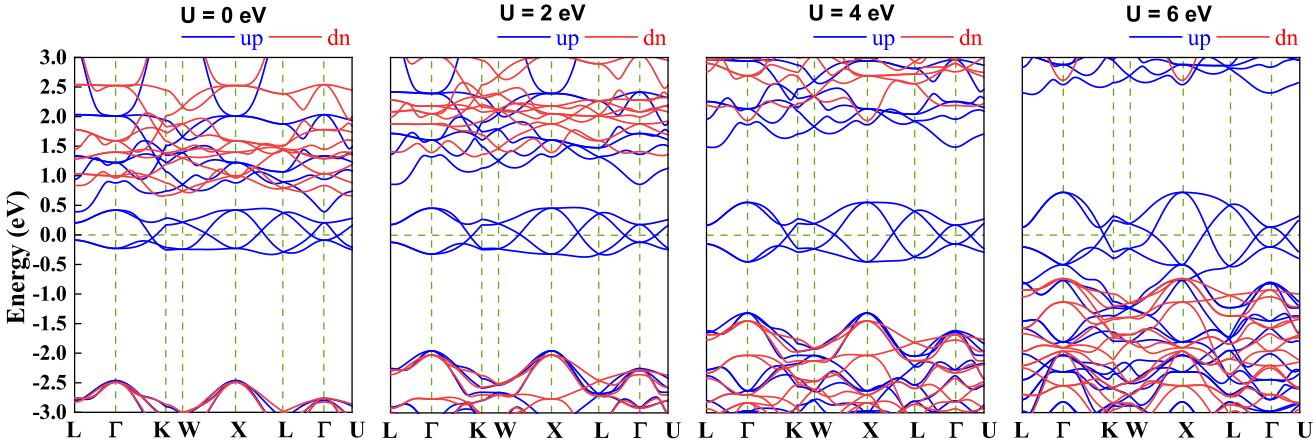

Figure S6: Band structures of VZn_2O_4 with the U_{eff} ranging from 0 to 6 eV.

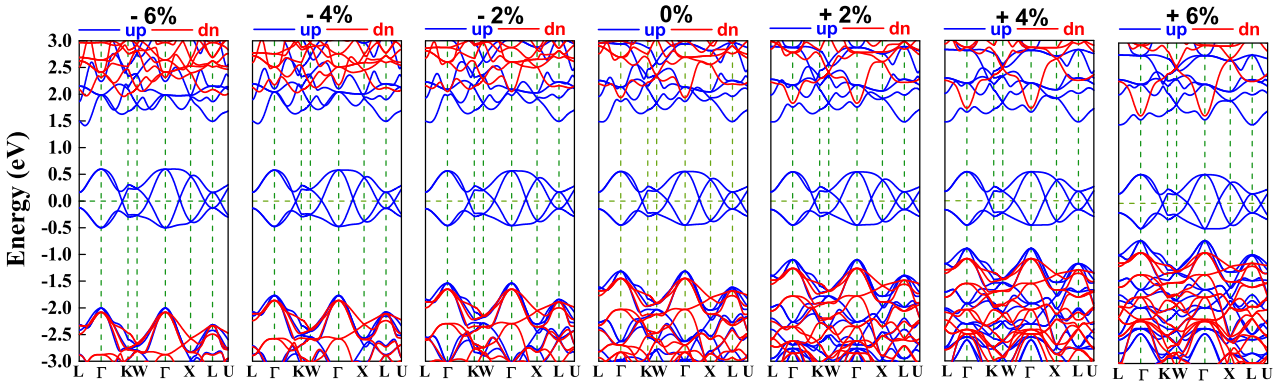

Figure S7: Band structures of VZn_2O_4 with additional strains ranging from -6% to +6%.

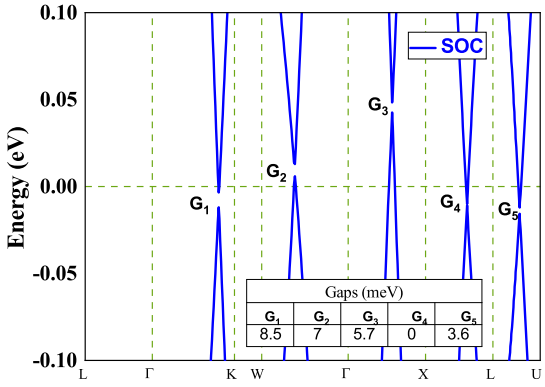

Figure S8: Band gaps with SOC for VZn_2O_4.

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