Supporting Information

High-throughput Screening of Stable Ag-Pd-F Catalysts for Formate Oxidation Reaction Using Machine Learning

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SUPPLEMENTARY METHODS

The crystal graph convolutional neural network (CGCNN) used in this study falls under the category of neural network algorithms. The core idea of CGCNN is to represent the crystal structure as a crystal graph, which encodes atomic information and interatomic bonding interactions, and then build a convolutional neural network on this graph. The model is trained using data from density functional theory (DFT) calculations to automatically extract representations that are most suitable for predicting the target properties.[1]

The crystal graph G is an undirected multigraph, where nodes represent atoms and edges represent the connections between atoms in the crystal. Unlike conventional graphs, the crystal graph allows multiple edges between the same pair of nodes, a feature that arises from the periodicity of crystals, thus distinguishing it from molecular graphs. Each node i is represented by a feature vector v_i, which encodes the properties of the atom corresponding to node i. The edge $(i,j)_k$ is represented by the feature vector $u_{(i,j)_k}$, which corresponds to the k-th bond connecting atom i and atom j.[1]

Atomic and bond properties are encoded using one-hot encoding in the node feature vector v_i and the edge feature vector $u_{(i,j)_k}$. For discrete values, the vector is encoded according to the category to which the value belongs; for continuous values, the range of attribute values is divided into 10 categories, and the vector is encoded accordingly. The atomic feature vector v_i includes 9 attributes: period, group, electronegativity, covalent radius, valence electrons, first ionization energy, electron affinity, block, and atomic volume. For example, if the atomic features are the group number and period number, the atomic feature vector for H will be a 27-dimensional vector, where the 1st and 19th elements are 1, and all other elements are 0. If the interatomic distance is 0.7, the bond feature vector will be a 10-dimensional vector, where the first element is 1, and all other elements are 0.[1]

Table S1 The different hyperparameter settings and performance of the CGCNN model. The partition ratio is a partition ratio of the training set, the validation set and the test set in the data set. The epoch is 100.

Composition	Symmetry	E_d (meV/atom)	Lattice parameters

The amount of training data	Partition ratio (%)	MAE (eV/atom)
42795	80：10：10	0.083
42975	60：20：20	0.088
65520	80：10：10	0.074
65520	60：20：20	0.079

Ag	$P6_3/mmc$	0	a = 2.91 b = 2.91 c = 9.46	α = β = 90° γ = 120°
Pd	$Fm\bar{3}m$	0	a = 3.92 b = 3.92 c = 3.92	α = β = γ = 90°
F	$C2/c$	0	a = 5.11 b = 3.17 c = 6.62	α = γ = 90° β = 94.87°
AgF	$Fm\bar{3}m$	0	a = 4.92 b = 4.92 c = 4.92	α = β = γ = 90°
AgF_2	$Pbca$	0	a = 5.15 b = 5.67 c = 5.74	α = β = γ = 90°
AgF_3	$P6_122$	0	a = 5.03 b = 5.03 c = 15.28	α = β = 90° γ = 120°
Ag_2F	$P\bar{3}m1$	0	a = 3.00 b = 3.00 c = 5.73	α = β = 90° γ = 120°
Ag_2F_5	$P\bar{1}$	0	a = 4.88 b = 7.36 c = 11.13	α = 88.62° β = 89.18° γ = 74.54°
AgPd	$R\bar{3}m$	0	a = 2.82 b = 2.82 c = 13.90	α = β = 90° γ = 120°
Ag_3Pd	$I4/mmm$	0	a = 4.07 b = 4.07 c = 8.04	α = β = γ = 90°
PdF_3	$R\bar{3}c$	0	a = 5.01 b = 5.01 c = 14.12	α = β = 90° γ = 120°
PdF_4	$Fdd2$	0	a = 5.72 b = 9.19 c = 9.42	α = β = γ = 90°
$AgPdF_6$	$P\bar{1}$	0	a = 4.95 b = 5.00 c = 10.04	α = 76.94° β = 77.44° γ = 61.01°

Table S2 The known Ag-Pd-F phases in the MP database, along with their space group symmetries, E_d values and lattice parameters.

Table S3 The CGCNN-1 model predicted 728 potentially stable Ag-Pd-F structures with 373 distinct Ag-Pd-F compositions, including potential stable structures， E_d values converted by E_f from CGCNN-1 model and E_d by DFT.

Composition	DFT-E_d (meV/atom)	CGCNN-E_d (meV/atom)	Composition	DFT-E_d (meV/atom)	CGCNN-E_d (meV/atom)
Ag_2PdF_6_La_2WO_6_2	-20.42	-43.855	$AgPd_9F_{27}$_$Na(WO_3)_9$_5	48.46	-225.188
Ag_2PdF_6_Na_2PdF_6_3	-19.78	-48.3778	$AgPd_3F_8$_$NaSb_3O_8$_3	48.83	-55.2145
$AgPd_2F_{12}$_$CaCr_2F_{12}$_2	-8.53	-156.148	$Ag_3Pd_2F_{12}$_$Y_2Cr_3O_{12}$_6	51.42	-23.5639
Ag_2PdF_6_Sm_2WO_6_2	-4.87	-10.6794	$Ag_2Pd_4F_{13}$_$Na_2W_4O_{13}$_5	51.75	-47.1596
$AgPd_2F_6$_Ca_2H_6Os_1	-4.66	-27.201	$Ag_2Pd_5F_{12}$_$Lu_5(ReO_6)_2$_3	52.14	-9.49922
$AgPd_4F_{10}$_ZrU_4O_{10}_4	10.73	-67.3089	$Ag_3Pd_2F_9$_$Pr_3Re_2O_9$_3	52.16	-28.6505
$AgPdF_5$_$CaCuF_5$_3	20.11	-65.779	$AgPdF_5$_$MgCuF_5$_3	52.67	-70.013
Ag_3PdF_7_Er_3TaO_7_3	27.43	-8.63915	Ag_3PdF_8_Ho_3ReO_8_3	53.15	-28.7498
$AgPdF_4$_$TbSbO_4$_6	28.33	-43.2003	$Ag_3Pd_{17}F_{47}$_$Sm_3Ta_{17}O_{47}$_2	54.50	-139.246
$Ag_4Pd_3F_{12}$_$Lu_4Hf_3O_{12}$_3	28.75	-6.26736	$Ag_2Pd_2F_7$_$Ta_2Pb_2O_7$_1	55.49	-40.4317
Ag_6PdF_{12}_La_6WO_{12}_2	29.27	-27.1889	$Ag_3Pd_4F_{13}$_$Nb_4Pb_3O_{13}$_1	55.70	-83.82
$AgPd_3F_7$_Er_3TaO_7_1	29.66	-21.8592	$AgPd_2F_6$_Tm_2TeO_6_1	56.29	-5.75549
Ag_3PdF_7_Sm_3MoO_7_1	29.86	-19.9782	$Ag_4Pd_2F_{15}$_$Dy_2Mo_4O_{15}$_3	57.85	-22.335
Ag_3PdF_{15}_$CaAs_3F_{15}$_4	33.99	-178.042	$Ag_6Pd_8F_{25}$_$Ta_8Pb_6O_{25}$_1	58.84	-84.8786
$Ag_3Pd_2F_{12}$_$Dy_2(SeO_4)_3$_3	34.36	-129.903	$AgPdF_4$_$EuSeO_4$_3	58.84	-9.45499
Ag_3PdF_7_Er_3SbO_7_3	36.22	-46.3002	$Ag_4Pd_6F_{19}$_$Ta_6Pb_4O_{19}$_1	59.61	-74.4805
Ag_2PdF_5_Na_2VF_5_3	36.97	-14.1475	$AgPdF_5$_$NbVO_5$_3	60.46	-106.071
$AgPd_4F_{12}$_$K(WO_3)_4$_2	37.02	-71.6163	$Ag_3Pd_{14}F_{28}$_$Ba_3(RhO_2)_{14}$_2	61.22	-16.8455
$Ag_2Pd_2F_7$_$Sm_2Mn_2O_7$_2	38.04	-184.797	$AgPd_6F_{18}$_$Rb(WO_3)_6$_5	61.46	-50.4212
$Ag_3Pd_2F_{12}$_$Ga_2(MoO_4)_3$_5	38.33	-46.3136	Ag_2PdF_7_Sr_2AlH_7_4	63.40	-65.1998
$Ag_3Pd_{10}F_{30}$_$Na_3(WO_3)_{10}$_5	42.72	-144.074	$Ag_5Pd_4F_{15}$_$Sr_5Ta_4O_{15}$_3	63.94	-57.2838
$AgPd_5F_{13}$_$NaSb_5O_{13}$_3	42.92	-86.2316	$AgPd_6F_{16}$_$BaTa_6O_{16}$_2	64.62	-108.172
$AgPd_{11}F_{33}$_$La(WO_3)_{11}$_2	43.08	-220.008	$Ag_3Pd_4F_{12}$_$Lu_4Hf_3O_{12}$_1	65.56	-11.5621
$Ag_3Pd_2F_{12}$_$Ho_2(SeO_4)_3$_3	43.53	-97.4793	Ag_4Pd_3F_Ti_4CN_3_4	66.43	-313.083
$AgPd_3F_9$_$Tl(WO_3)_3$_5	44.90	-79.1895	$AgPd_6F_{18}$_$Tl(WO_3)_6$_5	67.74	-100.531
$AgPd_2F_6$_Ta_2PbO_6_1	45.49	-101.813	$AgPdF_6$_$ZnFeF_6$_2	68.01	-151.424
$AgPd_2F_6$_$Ga(SiNi_3)_2$_4	46.16	-14.6001	$Ag_2Pd_2F_7$_$Tb_2Ti_2O_7$_4	68.03	-51.5722
$AgPd_7F_{19}$_$PrTa_7O_{19}$_3	46.29	-130.974	$AgPd_2F_{12}$_$CaAs_2F_{12}$_2	68.46	-256.909
$AgPd_3F_9$_$GdTa_3O_9$_3	46.74	-140.093	$AgPd_6F_{12}$_Lu_6TeO_{12}_3	69.19	-24.0946

The final number (i.e., _2) represent different atomic arrangement of the same substitution template (i.e., La_2WO_6)after substituting Ag, Pd, and F atoms.

$AgPd_3F_8$_Ho_3ReO_8_1	69.53	-48.5777	$Ag_3Pd_9F_{20}$_$Mg_3Ti_9O_{20}$_5	97.36	-63.7791
$Ag_5Pd_5F_{16}$_$La_5Mn_5O_{16}$_2	69.73	-74.8802	$Ag_2Pd_8F_{19}$_$U_8Bi_2O_{19}$_3	98.37	-8.61564
$Ag_7Pd_9F_{27}$_$Na_7(WO_3)_9$_5	69.88	-8.12305	$AgPdF_4$_$EuSeO_4$_1	99.37	-12.0826
$AgPdF_6$_$LiFeF_6$_6	71.39	-14.9831	$Ag_{12}Pd_8F_{27}$_$Sr_{12}Fe_8O_{27}$_3	99.45	-83.1198
$Ag_5Pd_2F_{12}$_$Tb_5(RuO_6)_2$_6	72.44	-12.0826	$AgPdF_5$_$ZnCuF_5$_3	99.55	-50.9413
$Ag_4Pd_3F_{12}$_$Mn_{12}Ge_4N_3$_3	74.88	-83.1198	$Ag_4Pd_4F_{13}$_$Ru_4Pb_4O_{13}$_1	100.99	-7.68368
$AgPd_{12}F_{33}$_$Ta_{12}MoO_{33}$_3	76.42	-162.607	$Ag_3Pd_3F_{11}$_$La_3Pt_3O_{11}$_1	102.06	-170.824
$AgPd_4F_8$_$NaTa_4O_8$_3	76.50	-9.21292	$Ag_{16}Pd_8F_{29}$_$Sr_{16}Mn_8O_{29}$_5	102.24	-44.5738
$Ag_4Pd_2F_9$_$Sr_4Ru_2O_9$_3	77.44	-90.9198	$Ag_3Pd_{16}F_{32}$_$Sr_3(RhO_2)_{16}$_5	103.22	-26.8075
Ag_3PdF_{12}_Cu_3SbF_{12}_1	81.41	-6.17149	$Ag_{28}Pd_{14}F_3$_$Ba_3(RhO_2)_{14}$_5	108.25	-63.498
$AgPdF_4$_$NaYF_4$_3	82.55	-28.4262	$AgPd_2F_5$_$TmMn_2O_5$_5	108.83	-185.458
$AgPdF_6$_$NaVF_6$_3	83.18	-129.149	$AgPd_5F_{10}$_$NaTi_5O_{10}$_5	108.94	-13.1986
$Ag_3Pd_3F_{10}$_$Tl_3Os_3O_{10}$_3	83.53	-21.0172	Ag_2PdF_6_Ca_2H_6Os_3	109.13	-58.9395
$Ag_{14}Pd_{10}F_{39}$_$Nb_{10}Pb_{14}O_{39}$_1	84.03	-84.4339	Ag_3Pd_5F_Li_5TiN_3_5	110.04	-148.501
$AgPd_8F_{16}$_$BaTi_8O_{16}$_2	85.26	-6.04457	$Ag_{15}Pd_{32}F_2$_$K_2Ta_{15}O_{32}$_5	110.09	-130.502
$Ag_3Pd_5F_{12}$_$La_3Sb_5O_{12}$_1	86.43	-48.0782	$Ag_2Pd_{15}F_{32}$_$K_2Ta_{15}O_{32}$_1	110.23	-44.784
$Ag_{21}Pd_{14}F_{47}$_$Sr_{21}Fe_{14}O_{47}$_3	86.51	-54.3525	$Ag_6Pd_7F_2$_$Li_6Hf_2O_7$_6	111.61	-46.1788
$Ag_5Pd_{13}F_{30}$_$Mg_5Ti_{13}O_{30}$_5	90.14	-74.326	$Ag_{32}Pd_{16}F_3$_$Rb_3Mn_{16}O_{32}$_2	111.71	-214.463
$AgPd_9F_{25}$_Nb_9VO_{25}_3	90.23	-21.5549	$Ag_3Pd_{20}F_{40}$_$Ba_3Ti_{20}O_{40}$_2	114.76	-16.3421
$AgPd_2F_6$_Tm_2WO_6_6	90.34	-82.0771	$Ag_{12}Pd_6F$_$Rb(IrO_2)_6$_6	114.92	-31.8258
$AgPdF_6$_$LiMnF_6$_4	90.48	-73.649	$Ag_2Pd_3F_7$_$Ca_3Fe_2O_7$_3	115.52	-38.4261
$AgPdF_3$_$YReN_3$_6	90.49	-51.9733	Ag_5Pd_4F_CeU_4N_5_5	116.45	-176.359
Ag_8Pd_3F_Ti_8Cu_3Ni_4	90.57	-9.13317	$Ag_{17}Pd_{12}F$_$Ti_{17}CuP_{12}$_6	116.95	-64.2842
Ag_3PdF_6_Ca_3WO_6_2	90.91	-80.4506	$Ag_7Pd_{12}F$_Mn_7GeO_{12}_6	118.10	-55.3586
$AgPd_2F_{12}$_$BaAs_2F_{12}$_2	92.35	-61.701	$Ag_{10}Pd_4F$_ZrU_4O_{10}_3	119.00	-7.56993
$AgPd_{13}F_{33}$_$NaNb_{13}O_{33}$_3	93.03	-0.087	Ag_3Pd_2F_Nb_3AlC_2_2	120.97	-186.84
$Ag_3Pd_{16}F_{32}$_$Rb_3Mn_{16}O_{32}$_5	93.68	-113.649	$AgPdF_4$_$ZnCrO_4$_4	121.91	-36.4862
$AgPd_3F_{12}$_Cu_3SbF_{12}_3	93.98	-96.9939	$AgPdF_3$_$LaAlO_3$_3	122.81	-223.579
Ag_2PdF_{12}_$CaCr_2F_{12}$_4	94.02	-80.2395	Ag_3Pd_8F_Ti_8Cu_3Ni_2	124.78	-43.5242
Ag_3PdF_6_Pr_3GaO_6_5	94.33	-66.3199	$Ag_{40}Pd_{20}F_3$_$Ba_3Ti_{20}O_{40}$_5	124.84	-9.61277
$AgPd_2F_6$_$Hg(SbO_3)_2$_1	94.76	-45.3916	$AgPdF_3$_$TaTlO_3$_3	125.37	-23.2981
$AgPd_6F_{12}$_$Rb(IrO_2)_6$_1	94.80	-139.27	$AgPd_8F_{14}$_$BaNb_8O_{14}$_3	129.25	-95.3692
$Ag_{12}Pd_8F_3$_$Al_3(V_3C_2)_4$_4	95.68	-67.3996	$AgPdF_3$_$GdInO_3$_1	129.35	-187.974

$Ag_2PdF_5\_Ce_2TiO_5\_2$	129.57	-136.435	$Ag_4Pd_8F\_Rb(RuO_2)_4\_5$	155.40	-138.346
$Ag_8Pd_{19}F_2\_U_8Bi_2O_{19}\_2$	130.14	-73.3638	$Ag_4Pd_{10}F\_ZrU_4O_{10}\_1$	156.93	-27.6176
$Ag_2Pd_7F_{16}\_Sr_2Zr_7O_{16}\_5$	131.27	-50.9413	$Ag_2Pd_2F_5\_Nd_2Pd_2O_5\_4$	159.14	-186.729
$Ag_{12}Pd_{17}F\_Ti_{17}CuP_{12}\_5$	131.27	-7.68368	$Ag_2Pd_{16}F\_Sm_2TiCo_{16}\_3$	160.15	-93.7587
$AgPd_2F_6\_YU_2O_6\_3$	131.48	-186.729	$Ag_7Pd_{12}F\_Y_7HoO_{12}\_2$	160.98	-72.1349
$Ag_6Pd_{23}F\_Zr_6Zn_{23}Si\_4$	132.60	-93.7587	$Ag_8Pd_3F\_TaSb_3O_8\_6$	161.09	-280.35
$Ag_4Pd_9F_2\_Mg_4Sb_2O_9\_5$	133.76	-105.041	$Ag_6Pd_8F\_Na_8CoO_6\_6$	162.14	-39.1154
$Ag_{19}Pd_{32}F_5\_Mg_5Co_{19}O_{32}\_2$	136.14	-46.6634	$Ag_5Pd_{12}F\_U_5ClO_{12}\_2$	163.39	-247.148
$Ag_3PdF_{12}\_Er(ReO_4)_3\_1$	136.51	-76.7524	$Ag_8Pd_4F\_Rb(RuO_2)_4\_6$	164.27	-15.0542
$Ag_6Pd_6F\_Hf_6Zn_6N\_6$	136.51	-6.733	$Ag_{14}Pd_4F\_Li_{14}MgSi_4\_4$	165.35	-225.423
$AgPd_6F\_EuZrF_6\_6$	136.98	-206.04	$Ag_9PdF_{27}\_Na(WO_3)_9\_6$	165.50	-2.44645
$Ag_2PdF_6\_Sr_2CuH_6\_4$	137.23	-147.775	$Ag_3Pd_{15}F\_LuZr_3F_{15}\_6$	165.57	-79.7658
$Ag_{11}Pd_8F\_Ti_{11}CuP_8\_6$	138.92	-57.9511	$Ag_{20}Pd_9F_3\_Mg_3Ti_9O_{20}\_2$	166.38	-92.4291
$Ag_5Pd_{16}F\_Ni_{16}GeP_5\_2$	139.22	-65.7131	$Ag_3Pd_{17}F_2\_Tm_2Fe_{17}C_3\_3$	166.75	-303.77
$Ag_{12}Pd_{37}F_2\_Al_{37}(Fe_6Cu)_2\_6$	140.97	-88.0762	$Ag_{19}Pd_8F_2\_U_8Bi_2O_{19}\_4$	167.68	-1.83543
$Ag_5Pd_{10}F\_NaTi_5O_{10}\_4$	142.22	-61.5011	$Ag_8Pd_{11}F\_Ti_{11}CuP_8\_5$	167.92	-51.1568
$Ag_9Pd_{39}F_2\_Al_2(Zn_{13}Pd_3)_3\_4$	142.85	-185.207	$Ag_6Pd_5F\_Li_5IO_6\_5$	168.57	-131.165
$Ag_{32}Pd_{21}F_3\_Co_{21}Cu_3O_{32}\_4$	143.02	-134.801	$Ag_{13}Pd_5F\_NaSb_5O_{13}\_4$	168.69	-77.3433
$Ag_{11}PdF_{33}\_La(WO_3)_{11}\_4$	143.42	-49.3241	$Ag_2Pd_5F_2\_Ba_2Sc_2O_5\_5$	169.22	-16.0313
$Ag_{33}Pd_{13}F\_NaNb_{13}O_{33}\_4$	144.05	-55.1175	$Ag_{15}Pd_3F\_Zr_3TlF_{15}\_5$	169.33	-119.635
$Ag_4PdF\_InSbO_4\_4$	145.67	-62.1171	$Ag_9Pd_2F\_CsU_2F_9\_6$	171.21	-247.613
$Ag_{14}Pd_{28}F_3\_Ba_3(RhO_2)_{14}\_6$	146.04	-351.317	$Ag_2Pd_7F_{15}\_Mg_2Ti_7O_{15}\_5$	171.26	-79.6034
$Ag_3Pd_{20}F\_BiSb_3F_{20}\_2$	146.85	-61.048	$Ag_{16}Pd_8F\_BaMn_8O_{16}\_5$	171.98	-156.032
$Ag_4Pd_2F\_Sr(RhO_2)_2\_2$	147.37	-12.2346	$Ag_3Pd_{15}F\_Zr_3TlF_{15}\_6$	172.66	-188.964
$Ag_3Pd_2F_7\_Ca_3Fe_2O_7\_1$	147.79	-41.8916	$Ag_4PdF_4\_Ca_4ZrN_4\_5$	173.81	-0.21635
$AgPd_7F_{12}\_Mn_7GeO_{12}\_2$	148.97	-119.056	$Ag_{12}Pd_2F\_BaSb_2F_{12}\_6$	174.26	-7.5345
$AgPd_2F_5\_Sc_2TiO_5\_4$	149.08	-243.101	$Ag_2Pd_{11}F\_NdHf_2F_{11}\_1$	174.76	-157.055
$Ag_5Pd_{13}F\_NaSb_5O_{13}\_2$	149.19	-73.2497	$Ag_{39}Pd_9F_2\_Al_2(Zn_{13}Pd_3)_3\_2$	175.91	-90.9663
$Ag_9Pd_9F\_Sc(TiN)_9\_5$	150.10	-378.699	$Ag_{19}Pd_{32}F_5\_Zn_5Co_{19}O_{32}\_2$	175.93	-87.852
$Ag_{16}Pd_8F\_Mn_8PbO_{16}\_5$	152.43	-87.9495	$AgPdF_4\_CoSi_4Ni\_4$	176.02	-51.0456
$Ag_{12}Pd_4F\_Mn_{12}Pt_4N\_6$	152.79	-145.05	$Ag_3Pd_{13}F\_U_3TlF_{13}\_2$	176.40	-197.226
$AgPd_2F_6\_Cs(OsO_3)_2\_3$	153.67	-42.9381	$Ag_4Pd_{12}F\_Mn_{12}Pt_4N\_5$	176.86	-108.329
$Ag_6Pd_3F_2\_Na_2Nb_3O_6\_4$	155.20	-2.11018	$Ag_{25}Pd_9F\_Nb_9VO_{25}\_4$	177.35	-88.585

$AgPd_3F_6$_$Ni(PtO_2)_3$_3	177.47	-36.2138	Ag_8Pd_2F_$BaLu_2F_8$_6	190.86	-57.4004
Ag_2PdF_$GaCuO_2$_5	178.70	-0.81872	$Ag_{10}Pd_3F$_Y_3TlF_{10}_6	191.59	-7.52956
Ag_2PdF_4_Eu_2TiO_4_2	178.80	-72.1349	Ag_9Pd_3F_$ErTa_3O_9$_4	191.67	-76.512
$Ag_{17}PdF$_$CeUZn_{17}$_5	179.29	-280.35	$Ag_{12}Pd_6F$_Lu_6WO_{12}_3	192.06	-32.751
$Ag_8Pd_{14}F$_$BaNb_8O_{14}$_2	179.32	-76.512	Ag_5Pd_3F_$RbIn_3O_5$_6	192.11	-146.646
$Ag_{12}Pd_5F_2$_$Y_5U_2O_{12}$_6	179.40	-32.751	Ag_2Pd_4F_Y_2HgO_4_5	192.37	-50.6997
Ag_7Pd_3F_Er_3TaO_7_6	180.77	-58.4261	Ag_4Pd_3F_Fe_3NiP_4_5	192.65	-173.734
$Ag_{23}Pd_6F$_$Zr_6Zn_{23}Si$_2	181.02	-46.5211	$AgPd_5F_{12}$_$LaSb_5O_{12}$_1	193.20	-203.665
Ag_5Pd_4F_Li_4WO_5_2	182.05	-1.55947	Ag_4Pd_2F_Co_2Mo_4N_4	193.38	-102.994
$Ag_{33}Pd_{12}F$_$Ta_{12}MoO_{33}$_4	182.28	-50.439	$Ag_{15}Pd_3F$_$LuZr_3F_{15}$_5	193.65	-449.295
$AgPd_3F_7$_Ta_3O_7F_3	182.31	-44.0388	Ag_9Pd_2F_NaU_2F_9_4	194.03	-132.817
$Ag_{27}Pd_4F_2$_$Al_{27}(FeNi_2)_2$_3	183.30	-135.39	Ag_5Pd_3F_Ti_5Si_3C_6	194.04	-140.792
$Ag_{10}Pd_3F$_$CsSc_3F_{10}$_4	184.33	-144.849	Ag_5Pd_2F_Sc_2TiO_5_3	195.08	-147.246
Ag_6PdF_8_Li_6NiCl_8_6	185.02	-24.2321	Ag_2PdF_$CuAuO_2$_6	195.69	-1.20392
Ag_3PdF_$FeSnO_3$_2	185.72	-33.5981	Ag_5PdF_5_Ca_5NbN_5_6	197.83	-220.301
Ag_4Pd_2F_MgV_2O_4_6	185.79	-72.8006	$Ag_{16}Pd_7F_2$_$Sr_2Zr_7O_{16}$_2	198.81	-16.3957
$Ag_9Pd_{25}F$_Nb_9VO_{25}_2	186.75	-22.1714	$Ag_{33}Pd_{11}F$_$La(WO_3)_{11}$_5	198.89	-100.383
$Ag_{11}Pd_{25}F_{60}$_$Mg_{11}Ti_{25}O_{60}$_5	187.32	-108.134	Ag_5Pd_5F_Li_5TaO_5_5	199.25	-104.999
$Ag_{27}Pd_{10}F_4$_$Y_{10}U_4O_{27}$_6	188.14	-50.2952	Ag_3Pd_8F_$TaSb_3O_8$_5	199.25	-248.025
$Ag_{10}Pd_6F$_$Nb_{10}Ge_6C$_1	188.28	-382.185	$Ag_{27}Pd_7F_9$_$Na_7(WO_3)_9$_1	199.36	-41.2104
$AgPd_2F_4$_$SrSc_2O_4$_3	188.38	-49.2118	$Ag_{47}Pd_{17}F_3$_$Sm_3Ta_{17}O_{47}$_5	200.11	-28.6526
$Ag_6Pd_{12}F$_$Rb(IrO_2)_6$_5	188.67	-92.2219	$Ag_2Pd_{14}F$_$Y_2Fe_{14}C$_5	200.23	-376.015
$Ag_{27}Pd_9F$_$Na(WO_3)_9$_2	188.79	-64.0385	Ag_7PdF_$LuPtF_7$_6	200.56	-11.1168
Ag_2Pd_7F_$InPb_2F_7$_1	189.37	-224.212	$Ag_2Pd_2F_{11}$_$Ta_2Mo_2O_{11}$_3	201.92	-127.655
Ag_4Pd_5F_Li_5AuO_4_5	189.51	-5.50317	$AgPd_7F$_$LuHfF_7$_2	201.98	-138.162
Ag_6Pd_3F_Ta_3NO_6_6	189.57	-46.401	$AgPdF_4$_$GdAsO_4$_6	202.00	-225.835
$AgPd_2F_5$_Lu_2TiO_5_4	189.65	-37.4264	$Ag_6Pd_{11}F_5$_$Zn_6B_5Ir_{11}$_2	202.13	-160.692
Ag_2PdF_$CrAuO_2$_5	190.05	-89.0534	Ag_4Pd_3F_$LiTa_3N_4$_1	202.28	-26.8036
Ag_2Pd_5F_Lu_2TiO_5_1	190.15	-156.023	$AgPd_4F$_$KGdF_4$_2	202.30	-32.3361
Ag_3Pd_2F_Li_2IrO_3_2	190.42	-208.024	$Ag_{12}Pd_5F_2$_$Lu_5(ReO_6)_2$_4	202.56	-233.639
$Ag_{10}Pd_5F$_$NaTi_5O_{10}$_2	190.55	-77.2326	Ag_2Pd_6F_YU_2O_6_2	203.04	-29.5574
$AgPd_2F_4$_Y_2HgO_4_1	190.55	-72.1971	$Ag_{15}PdF_3$_$LuZr_3F_{15}$_3	203.56	-33.1499
Ag_9Pd_9F_$Sc(TiN)_9$_6	190.71	-44.4881	$Ag_{10}Pd_{27}F_4$_$Y_{10}U_4O_{27}$_5	203.59	-216.42

$Ag_{19}Pd_7F\_PrTa_7O_{19}\_4$	204.27	-80.7474	$AgPd_7F\_LuZrF_7\_1$	215.49	-13.2492
$AgPd_2F_4\_Sr(RhO_2)_2\_5$	204.50	-105.203	$Ag_{57}Pd_{17}F_{19}\_Na_{17}(WO_3)_{19}\_1$	215.57	-242.378
$AgPd_2F_4\_SrNb_2O_4\_3$	205.03	-291.572	$Ag_{37}Pd_{12}F_2\_Al_{37}(Fe_6Cu)_2\_5$	215.66	-98.0154
$Ag_6Pd_{21}F_2\_Ni_{21}(GeB_3)_2\_5$	205.35	-146.646	$Ag_{20}Pd_3F\_BiSb_3F_{20}\_4$	215.84	-47.4357
$Ag_4Pd_2F\_Y_2HgO_4\_6$	205.50	-98.0154	$AgPd_{14}F_2\_Y_2Fe_{14}C\_2$	216.26	-70.3745
$Ag_7PdF\_LuZrF_7\_3$	205.54	-47.4357	$Ag_6Pd_2F\_Na_2CeF_6\_6$	216.71	-31.7872
$Ag_4Pd_2F\_SrNb_2O_4\_4$	205.66	-233.762	$Ag_3Pd_8F\_NaSb_3O_8\_2$	216.74	-141.239
$Ag_6PdF\_ZnCrF_6\_5$	206.43	-81.1883	$Ag_4Pd_2F\_Ca(AgO_2)_2\_6$	216.92	-57.1278
$Ag_9Pd_4F_2\_Mg_4Sb_2O_9\_6$	207.28	-37.9809	$Ag_6Pd_2F\_K_2SnF_6\_3$	217.35	-68.1588
$Ag_2Pd_6F\_Ni(IO_3)_2\_2$	207.42	-1.34899	$Ag_{12}Pd_7F\_Y_7HoO_{12}\_4$	217.50	-163.293
$Ag_7Pd_2F\_InPb_2F_7\_3$	207.78	-66.8612	$Ag_2Pd_3F\_Na_2PdO_3\_5$	218.26	-17.1154
$Ag_6Pd_2F\_LiCu_2F_6\_3$	207.82	-288.595	$Ag_3Pd_4F\_LiTa_3N_4\_3$	218.50	-38.2704
$Ag_5Pd_{12}F_2\_Lu_5(ReO_6)_2\_2$	207.87	-76.4566	$Ag_2Pd_7F_{12}\_U_2Co_{12}P_7\_6$	219.34	-86.7713
$Ag_{12}Pd_4F_3\_Lu_4Hf_3O_{12}\_6$	208.17	-122.112	$Ag_3Pd_2F\_Mg_2NbN_3\_2$	219.59	-61.6421
$Ag_4Pd_5F\_Na_5FeO_4\_4$	208.22	-29.6253	$Ag_7Pd_2F\_KTm_2F_7\_5$	219.64	-137.693
$Ag_5Pd_6F\_Li_5OsO_6\_6$	208.37	-82.0838	$Ag_3Pd_7F\_Er_3TaO_7\_5$	220.77	-103.329
$Ag_6PdF\_BaIrF_6\_3$	209.12	-49.2166	$Ag_4Pd_5F\_Li_4WO_5\_4$	220.95	-34.4964
$Ag_{16}Pd_6F_5\_Mg_6Te_5O_{16}\_6$	210.05	-179.091	$Ag_{12}Pd_5F\_U_5ClO_{12}\_4$	221.12	-84.8178
$Ag_5Pd_8F\_Co_5SbO_8\_2$	210.12	-117.256	$AgPd_7F\_LuPtF_7\_2$	221.55	-19.4336
$Ag_7Pd_6F\_Li_7BiO_6\_4$	210.55	-62.2568	$Ag_2Pd_4F\_Ni(AsO_2)_2\_4$	222.68	-1.53055
$Ag_7PdF\_BaWF_7\_3$	211.08	-201.194	$Ag_{12}PdF\_MnAl_{12}Fe\_2$	223.63	-200.8
$Ag_4Pd_3F\_Ti_4GaC_3\_4$	211.18	-73.1576	$Ag_3Pd_6F\_Li_3FeF_6\_4$	223.82	-342.572
$Ag_7Pd_{31}F_6\_Zr_6Ag_7F_{31}\_1$	211.58	-32.1621	$Ag_{27}Pd_9F_8\_Ba_9Rh_8O_{27}\_3$	224.10	-27.7994
$Ag_{15}PdF_3\_Zr_3TlF_{15}\_3$	211.72	-209.998	$Ag_7Pd_3F\_Na_3CeF_7\_6$	224.30	-0.93723
$Ag_{79}Pd_{22}F_{10}\_K_{10}Gd_{22}F_{79}\_6$	211.80	-65.1588	$AgPdF_3\_CaH_3Pd\_3$	224.40	-189.205
$AgPd_4F_4\_Th(BOs)_4\_6$	212.27	-85.3583	$Ag_{17}Pd_{47}F_3\_Sm_3Ta_{17}O_{47}\_6$	224.48	-68.743
$Ag_3Pd_8F\_Ho_3ReO_8\_5$	212.63	-74.6606	$AgPd_2F_5\_Ti_2CoO_5\_2$	224.50	-127.372
$Ag_6Pd_{12}F\_Lu_6TeO_{12}\_2$	213.20	-315.678	$Ag_9Pd_{60}F_{20}\_K_9(WO_3)_{20}\_1$	224.67	-112.685
$AgPd_9F_2\_NaU_2F_9\_5$	214.63	-66.5408	$Ag_5Pd_4F\_Li_5AuO_4\_6$	224.92	-26.114
$Ag_2Pd_6F\_Tm_2WO_6\_3$	214.70	-34.4413	$Ag_5Pd_4F\_Na_5FeO_4\_2$	225.15	-152.496
$Ag_{21}Pd_2F_5\_Dy_2Au_5F_{21}\_6$	215.09	-6.2665	$Ag_8Pd_4F\_CaNb_4O_8\_4$	225.81	-6.6502
$Ag_2Pd_6F\_Nb_2CdO_6\_5$	215.16	-197.532	$Ag_{13}Pd_3F\_U_3TlF_{13}\_4$	226.57	-33.0538
$Ag_6PdF\_LiWF_6\_5$	215.29	-248.274	$AgPdF_3\_ScGaO_3\_4$	227.19	-64.0804

$Ag_{16}Pd_5F_5$_$La_5Mn_5O_{16}$_3	227.56	-38.5266	$Ag_{60}Pd_{25}F_{11}$_$Mg_{11}Ti_{25}O_{60}$_2	243.02	-120.07
$Ag_8Pd_3F_2$_$Mg_2Mn_3O_8$_2	227.76	-59.1424	$AgPd_{15}F_3$_$LuZr_3F_{15}$_1	243.51	-76.7728
$Ag_2Pd_3F_8$_$Ca_2V_3O_8$_1	228.04	-17.0943	Ag_2Pd_5F_Ti_2CoO_5_6	244.26	-45.4478
Ag_3Pd_2F_Li_2RhO_3_5	228.63	-70.3745	Ag_9Pd_2F_KPu_2F_9_6	245.03	-88.5688
$Ag_2Pd_{17}F_2$_$Ce_2Mn_{17}C_2$_2	228.74	-88.5688	Ag_2Pd_6F_Sb_2WO_6_3	245.11	-21.8024
$Ag_9Pd_4F_2$_$Ca_4Ta_2O_9$_3	229.33	-150.9	Ag_2Pd_9F_NaU_2F_9_2	245.26	-169.867
$Ag_{13}Pd_{33}F$_$NaNb_{13}O_{33}$_2	229.41	-76.3499	Ag_3PdF_6_$Ni(PtO_2)_3$_1	245.42	-169.502
$Ag_2Pd_{27}F_4$_$Al_{27}(FeNi_2)_2$_6	230.18	-21.5069	$Ag_{32}Pd_{16}F_3$_$Sr_3(RhO_2)_{16}$_2	245.51	-31.0111
$Ag_9Pd_{20}F_3$_$Mg_3Ti_9O_{20}$_4	230.19	-35.4435	$Ag_7Pd_{27}F_9$_$Na_7(WO_3)_9$_3	245.80	-36.1462
$AgPd_3F_7$_Lu_3SbO_7_3	230.47	-410.865	$AgPd_5F$_$CeTlF_5$_5	245.80	-87.784
$Ag_{12}Pd_7F_2$_$Co_7(SbO_6)_2$_4	230.61	-81.569	$Ag_2Pd_7F_2$_$Ta_2Pb_2O_7$_2	246.36	-22.8747
$Ag_3Pd_{10}F$_Y_3TlF_{10}_5	231.20	-69.5255	$AgPdF_4$_$NaErF_4$_1	246.55	-209.054
$Ag_6Pd_{16}F$_$BaTa_6O_{16}$_6	231.50	-104.025	$AgPd_{17}F$_$SmGdCo_{17}$_3	246.79	-51.7456
Ag_2Pd_2F_Zr_2N_2O_2	231.62	-18.1605	Ag_2Pd_4F_Cd_2PbO_4_2	247.97	-30.6302
$Ag_5Pd_{12}F_2$_$Y_5U_2O_{12}$_5	232.05	-166.714	Ag_7PdF_$LuHfF_7$_4	248.51	-61.5528
Ag_5Pd_3F_Li_5TiN_3_6	232.49	-252.104	Ag_6PdF_2_$Ni(BiO_3)_2$_6	249.91	-199.79
Ag_2Pd_3F_$NbZn_2N_3$_4	232.51	-13.9012	Ag_5Pd_4F_Li_5OsN_4_4	250.05	-258.617
$Ag_{16}Pd_7F_5$_$Li_5Mn_7O_{16}$_1	234.36	-52.5709	Ag_8Pd_2F_BaY_2F_8_6	250.21	-39.8305
$Ag_8Pd_5F_2$_$Sr_5(AuO_4)_2$_6	234.41	-46.3477	$AgPd_{15}F_3$_Zr_3TlF_{15}_1	250.55	-286.947
$Ag_{12}Pd_4F_3$_$Lu_4Zr_3O_{12}$_3	234.92	-167.862	Ag_8Pd_5F_$BaNb_5O_8$_4	251.30	-28.4374
Ag_4Pd_3F_Mg_3MoN_4_5	235.01	-30.3173	$Ag_{15}Pd_{17}F_6$_$Zn_{15}B_6Rh_{17}$_2	251.53	-108.766
Ag_6Pd_2F_$Ni(IO_3)_2$_4	235.99	-218.835	$Ag_3Pd_{10}F_2$_$La_3U_2O_{10}$_5	251.80	-25.2155
$AgPd_{20}F_3$_$BiSb_3F_{20}$_5	236.11	-187.547	$Ag_{12}Pd_5F_4$_$Li_4Mn_5O_{12}$_1	252.30	-49.6729
$AgPd_2F$_$ZnMoN_2$_4	236.59	-37.9337	Ag_7PdF_$LuPtF_7$_4	253.01	-218.173
$Ag_{21}Pd_6F_2$_$Cr_{21}(WC_3)_2$_4	236.70	-107.909	$Ag_4Pd_{17}F_3$_$Sr_4Lu_3F_{17}$_6	253.26	-19.098
$AgPd_4F$_$NbGaO_4$_6	237.54	-22.8039	Ag_2Pd_3F_Mg_2ReN_3_4	253.32	-122.845
Ag_6PdF_$BaHfF_6$_3	238.25	-365.682	$AgPdF_4$_$GdYH_4$_4	253.84	-186.765
$Ag_3Pd_{15}F$_Zr_3InF_{15}_4	238.58	-162.002	$Ag_{17}Pd_8F_3$_$K_3Ti_8O_{17}$_5	254.09	-100.626
Ag_2Pd_6F_Tm_2TeO_6_5	240.01	-96.1291	Ag_3Pd_2F_Li_2PtO_3_5	254.74	-17.4412
$AgPd_2F$_$CrAuO_2$_6	240.56	-76.9975	$Ag_3Pd_5F_{12}$_$La_3Ga_5O_{12}$_2	255.65	-36.1971
$Ag_{10}Pd_3F$_KLu_3F_{10}_6	241.07	-85.8935	$AgPd_7F$_$LuPtF_7$_5	259.10	-98.78
$Ag_7Pd_{12}F_2$_$U_2Co_{12}P_7$_3	241.60	-22.5405	$Ag_3Pd_{12}F_4$_$Lu_4Hf_3O_{12}$_2	259.74	-242.992
$Ag_5Pd_{15}F_4$_$Sr_5Nb_4O_{15}$_5	241.63	-266.019	$AgPd_7F$_$BaWF_7$_1	259.84	-63.0038

$Ag_2Pd_2F_7$_$Y_2Pt_2O_7$_1	259.99	-122.832	Ag_6Pd_3F_Na_3InF_6_4	272.84	-83.3383
$Ag_9Pd_{28}F_5$_$Y_9U_5O_{28}$_5	261.24	-106.237	$Ag_4Pd_{12}F_3$_$Lu_4Hf_3O_{12}$_5	273.80	-14.9087
Ag_2Pd_6F_Li_2SnF_6_6	261.39	-68.7846	Ag_3Pd_4F_Ti_4GaC_3_2	274.42	-153.03
$Ag_{17}Pd_2F_2$_$Th_2Mn_{17}C_2$_6	261.45	-21.8024	$Ag_9Pd_{30}F_{10}$_$Ba_9Nb_{10}O_{30}$_5	275.57	-156.49
$Ag_{11}Pd_{24}F_7$_$Li_7Ti_{11}O_{24}$_1	261.57	-156.49	$AgPd_{12}F$_$MnAl_{12}Fe$_4	276.08	-270.221
$Ag_{16}Pd_{39}F_{12}$_$Sr_{16}V_{12}O_{39}$_5	262.12	-177.03	Ag_2Pd_6F_Li_2AgF_6_6	276.32	-23.6659
$AgPdF_2$_$SrCuO_2$_3	262.16	-136.515	$Ag_5Pd_{12}F_3$_$Dy_3Y_5O_{12}$_5	276.51	-48.7679
$Ag_{11}Pd_4F_4$_$Ba_4Fe_4O_{11}$_4	263.53	-55.4561	Ag_3Pd_5F_Ti_5Si_3C_5	276.92	-50.4749
$Ag_{11}PdF_2$_$NdHf_2F_{11}$_5	263.89	-6.21723	Ag_2PdF_8_$Mg(ReO_4)_2$_1	277.15	-104.763
Ag_2Pd_4F_MgV_2O_4_5	264.34	-35.6865	Ag_2Pd_4F_$SrNb_2O_4$_2	277.48	-93.479
$Ag_{32}Pd_{15}F_2$_$K_2Ta_{15}O_{32}$_6	264.86	-186.441	Ag_2PdF_{12}_$CaAs_2F_{12}$_4	277.76	-141.222
$Ag_3Pd_6F_2$_$Na_2Nb_3O_6$_2	265.22	-158.753	$Ag_{16}Pd_{32}F_3$_$Sr_3(RhO_2)_{16}$_4	278.15	-162.077
$Ag_{11}Pd_{104}F_{30}$_$Ta_{11}(Co_{52}B_{15})_2$_3	265.47	-196.521	$Ag_3Pd_{14}F$_Pr_3MgNi_{14}_4	278.79	-213.02
Ag_4Pd_3F_Li_3RuO_4_2	266.02	-125.55	$AgPd_8F_3$_$NaSb_3O_8$_5	279.30	-108.997
$Ag_{17}Pd_{57}F_{19}$_$Na_{17}(WO_3)_{19}$_3	267.50	-164.305	$Ag_5Pd_3F_{12}$_$Lu_3Sb_5O_{12}$_3	279.34	-46.5239
$AgPd_{14}F_8$_$BaNb_8O_{14}$_5	267.68	-40.2011	Ag_5Pd_5F_Li_5TaO_5_6	279.90	-173.357
Ag_3PdF_Ti_3ZnN_6	267.87	-240.754	$Ag_3Pd_{10}F$_$GaNi_{10}P_3$_1	280.22	-94.2098
$Ag_{10}Pd_9F_4$_$Na_{10}Zn_4O_9$_5	267.97	-20.7267	Ag_4PdF_$MgTeO_4$_4	280.65	-60.7341
$Ag_6Pd_{10}F$_$V_{10}Si_6B$_2	268.38	-112.244	$Ag_{15}Pd_5F_4$_$Sr_5Nb_4O_{15}$_6	282.21	-187.425
Ag_2Pd_3F_$MgTa_2N_3$_3	269.09	-167.509	Ag_2Pd_2F_Hf_2N_2O_1	282.82	-23.656
$Ag_6Pd_{11}F_3$_$La_6Ga_3Co_{11}$_3	269.25	-151.665	$Ag_3Pd_9F_2$_$Nd_3Re_2O_9$_6	282.88	-43.3503
$Ag_4Pd_9F_2$_$Ca_4Ta_2O_9$_1	269.30	-169.19	$Ag_{14}Pd_2F$_$Y_2Fe_{14}C$_6	283.18	-88.5901
Ag_3Pd_8F_Ta_3Mn_8Al_2	269.46	-282.237	$Ag_7Pd_{15}F_2$_$Mg_2Ti_7O_{15}$_4	283.82	-58.7183
$Ag_{12}Pd_{33}F$_$Ta_{12}MoO_{33}$_2	269.54	-49.7953	Ag_2Pd_5F_K_2LuF_5_2	284.31	-40.9337
$Ag_{12}Pd_7F$_Mn_7GeO_{12}_5	269.78	-46.5234	Ag_4Pd_5F_Li_5OsN_4_2	285.24	-65.3635
$Ag_{14}Pd_8F$_$BaNb_8O_{14}$_4	269.78	-223.258	Ag_3Pd_8F_Zr_3AlFe_8_6	285.41	-6.09693
$Ag_5Pd_{16}F_5$_$La_5Mn_5O_{16}$_1	270.96	-175.845	Ag_8Pd_6F_Na_8CoO_6_5	285.44	-231.923
$Ag_6Pd_{17}F_3$_$Sm_6U_3O_{17}$_2	271.03	-94.0328	$AgPd_4F$_$InSbO_4$_5	285.77	-29.7424
$Ag_{32}Pd_{19}F_5$_$Mg_5Co_{19}O_{32}$_4	271.45	-64.6279	Ag_4Pd_2F_AlV_2O_4_6	286.43	-222.105
Ag_4Pd_2F_Cd_2PbO_4_4	272.14	-16.6244	Ag_2Pd_8F_$BaLu_2F_8$_5	287.21	-220.451
$AgPd_{10}F_3$_$CsSc_3F_{10}$_5	272.38	-7.88562	Ag_2Pd_7F_KTm_2F_7_6	287.28	-213.548
$AgPd_4F$_$NaYF_4$_2	272.57	-52.0381	$Ag_2Pd_{32}F_{15}$_$K_2Ta_{15}O_{32}$_2	287.34	-14.2512
$Ag_7Pd_{16}F_2$_$Sr_2Zr_7O_{16}$_4	272.62	-96.6174	$Ag_9Pd_{27}F_8$_$Ba_9Rh_8O_{27}$_1	287.84	-136.808

$Ag_2Pd_5F\_Na_2VF_5\_5$	287.93	-132.332	$AgPd_6F\_CuPdF_6\_6$	303.07	-5.64407
$Ag_{13}Pd_{30}F_5\_Mg_5Ti_{13}O_{30}\_4$	288.93	-56.2031	$Ag_5Pd_6F_2\_Sc_6N_2O_5\_4$	303.78	-11.4766
$AgPd_4F\_MgTeO_4\_2$	289.28	-270.221	$AgPd_{10}F_3\_CsLu_3F_{10}\_2$	303.99	-262.362
$AgPd_2F\_Ti_2CN\_5$	289.33	-23.6659	$Ag_{24}Pd_{15}F_4\_Ti_4(Ni_5O_8)_3\_1$	305.48	-157.867
$Ag_2Pd_3F\_Li_2IrO_3\_4$	289.40	-35.9554	$Ag_2Pd_6F\_K_2SnF_6\_1$	305.91	-128.21
$Ag_{30}Pd_9F_{10}\_Ba_9Nb_{10}O_{30}\_6$	289.49	-116.078	$Ag_3Pd_9F\_ErTa_3O_9\_2$	306.22	-77.3583
$Ag_2PdF\_ScTaN_2\_4$	290.06	-10.4151	$Ag_2PdF\_ZnMoN_2\_2$	306.98	-76.2225
$Ag_2Pd_{17}F_2\_Ce_2Mn_{17}C_2\_5$	290.25	-178.987	$Ag_3Pd_{10}F\_KLu_3F_{10}\_5$	307.02	-86.7424
$AgPd_{10}F_3\_KLu_3F_{10}\_2$	290.29	-121.782	$AgPd_3F\_FeSnO_3\_4$	307.09	-336.55
$AgPd_4F\_LiAgF_4\_1$	290.55	-71.1739	$Ag_3Pd_5F\_Li_5GeN_3\_2$	307.13	-202.655
$Ag_3Pd_4F\_Li_3RuO_4\_4$	290.78	-112.261	$Ag_6Pd_7F\_Li_7BiO_6\_2$	307.63	-2.33652
$Ag_3PdF\_NbOF_3\_5$	291.05	-90.6089	$AgPd_4F\_InSbO_4\_2$	308.12	-33.3901
$Ag_2PdF\_ScTaN_2\_6$	291.81	-212.573	$AgPd_9F_2\_CsU_2F_9\_2$	309.24	-203.366
$AgPd_{10}F_3\_Y_3TlF_{10}\_2$	291.84	-172.799	$AgPd_3F\_NbOF_3\_6$	309.35	-127.218
$Ag_{20}Pd_{40}F_3\_Ba_3Ti_{20}O_{40}\_6$	293.93	-117.793	$AgPd_3F_2\_MgTa_2N_3\_4$	309.35	-14
$Ag_9Pd_3F_2\_Ba_3Re_2O_9\_4$	295.65	-4.95753	$AgPd_3F\_Ti_3ZnN\_5$	309.39	-15.7297
$AgPd_9F_3\_ErTa_3O_9\_5$	295.70	-45.6385	$Ag_4Pd_{11}F_4\_Ba_4Fe_4O_{11}\_2$	309.82	-162.593
$AgPd_4F\_LiAgF_4\_6$	296.58	-4.52607	$Ag_6Pd_{25}F\_KTh_6F_{25}\_5$	311.20	-140.185
$AgPd_6F\_LiWF_6\_6$	296.76	-120.219	$Ag_2Pd_5F\_Sc_2TiO_5\_1$	311.56	-52.9845
$AgPd_5F\_HfTlF_5\_5$	296.85	-87.9126	$AgPd_{13}F_3\_U_3TlF_{13}\_5$	313.04	-90.9605
$Ag_2Pd_2F_5\_Nd_2Pd_2O_5\_2$	297.37	-98.9083	$Ag_7Pd_2F\_KIn_2F_7\_5$	313.24	-90.3729
$Ag_8Pd_5F\_Co_5SbO_8\_4$	297.82	-137.467	$AgPd_6F_2\_Ni(BiO_3)_2\_5$	314.08	-248.027
$Ag_8Pd_{12}F_3\_Al_3(V_3C_2)_4\_2$	298.68	-37.3657	$Ag_3Pd_{12}F_4\_Lu_4Zr_3O_{12}\_6$	314.32	-121.672
$Ag_2Pd_6F\_Na_2CeF_6\_5$	299.96	-0.75534	$Ag_2Pd_6F\_Na_2UF_6\_5$	314.49	-110.376
$Ag_7Pd_{12}F_2\_Co_7(SbO_6)_2\_2$	300.20	-185.045	$Ag_7Pd_2F_2\_Ba_2Ta_2O_7\_3$	315.07	-355.684
$Ag_7Pd_3F\_La_3SbO_7\_4$	300.51	-45.9946	$Ag_6Pd_4F\_Na_6ZnO_4\_5$	315.12	-42.6554
$Ag_2Pd_4F\_Al_2CoO_4\_5$	300.70	-150.737	$Ag_4PdF\_CuTeO_4\_6$	315.63	-26.3495
$AgPd_7F_2\_KTm_2F_7\_1$	301.13	-27.6994	$Ag_{15}Pd_3F\_Zr_3InF_{15}\_2$	315.78	-43.1694
$Ag_6Pd_{16}F_5\_Mg_6Te_5O_{16}\_5$	301.21	-100.091	$Ag_6Pd_{31}F_7\_Zr_6Ag_7F_{31}\_6$	316.00	-210.804
$Ag_2Pd_{10}F\_Lu(Fe_5Si)_2\_2$	301.32	-18.2977	$Ag_3Pd_6F\_Na_3InF_6\_2$	317.30	-134.613
$Ag_{10}Pd_3F\_CsLu_3F_{10}\_6$	301.78	-262.162	$Ag_2Pd_{13}F_4\_Sm_2Fe_4Co_{13}\_3$	318.47	-0.65937
$AgPd_4F_2\_Co_2SnO_4\_6$	301.95	-26.8573	$Ag_5Pd_{19}F_3\_Fe_3Pb_5F_{19}\_1$	318.49	-130.086
$Ag_3Pd_3F_2\_Hf_3N_2O_3\_6$	302.31	-224.609	$Ag_2Pd_{17}F_3\_Tm_2Fe_{17}C_3\_4$	318.51	-79.2289

$AgPd_8F_5$_$BaNb_5O_8$_5	320.57	-128.21	$AgPd_5F$_$HfGa_5Co$_5	341.91	-42.5243
$AgPd_4F$_$CuTeO_4$_2	321.51	-77.3583	Ag_2Pd_3F_Mg_2NbN_3_4	342.62	-99.4102
$AgPd_6F$_$BaIrF_6$_1	321.57	-76.2225	$Ag_{11}Pd_{18}F_8$_$Zn_{11}(B_4Rh_9)_2$_2	343.19	-9.77037
Ag_7Pd_4F_Sm_4PdO_7_6	322.30	-86.7424	Ag_2Pd_6F_Hf_2BIr_6_2	343.72	-198.455
$AgPd_2F_4$_$Cd(GaO_2)_2$_2	322.45	-152.668	$Ag_{25}Pd_{60}F_{11}$_$Mg_{11}Ti_{25}O_{60}$_4	345.47	-25.3447
Ag_2Pd_9F_La_2AlNi_9_5	324.32	-12.2803	Ag_3PdF_$ThTaN_3$_2	345.49	-43.4126
Ag_2Pd_4F_Co_2Mo_4N_2	324.34	-0.77021	$Ag_{10}Pd_{79}F_{22}$_$K_{10}Gd_{22}F_{79}$_2	345.72	-11.6212
Ag_2Pd_9F_AlV_9Au_2_2	324.87	-106.466	$Ag_{25}Pd_6F$_KTh_6F_{25}_6	346.45	-202.224
$Ag_{12}Pd_6F$_$RbMn_6O_{12}$_2	325.35	-202.589	$AgPd_4F$_$LiVF_4$_1	347.17	-208.272
Ag_4Pd_2F_Ga_2CoO_4_5	325.50	-19.4307	$AgPd_3F$_$LaNi_3B$_2	347.91	-5.47384
$Ag_{20}PdF_3$_$BiSb_3F_{20}$_6	326.12	-210.796	$Ag_6Pd_{20}F_3$_$Nb_3(Ni_{10}B_3)_2$_5	347.97	-143.93
Ag_4Pd_8F_$CaNb_4O_8$_2	328.38	-22.2775	Ag_2PdF_6_Ni_6Ge_2B_1	348.67	-42.258
$Ag_5Pd_8F_2$_$Sr_5(AuO_4)_2$_5	329.61	-81.0517	$Ag_{16}Pd_{32}F_3$_$Rb_3Mn_{16}O_{32}$_4	348.86	-135.539
Ag_3Pd_6F_Li_3NiF_6_4	330.45	-186.305	Ag_8Pd_3F_$NaSb_3O_8$_4	355.49	-147.506
Ag_2Pd_3F_U_2Fe_3Si_5	330.47	-146.271	Ag_2Pd_4F_$Sr(RhO_2)_2$_4	355.50	-37.3217
$AgPd_8F_2$_$BaLu_2F_8$_2	330.50	-41.4909	$Ag_3Pd_{10}F_2$_$Y_3U_2O_{10}$_5	356.43	-160.073
$AgPd_8F_2$_BaY_2F_8_2	331.39	-47.1606	$Ag_3Pd_5F_2$_$Mg_3B_2Rh_5$_5	356.67	-225.034
$AgPd_3F_4$_$SrPt_3O_4$_3	331.55	-173.302	$Ag_{32}Pd_{35}F$_$FeNi_{35}S_{32}$_3	356.87	-113.304
$AgPd_3F$_$TiVO_3$_3	332.58	-79.3456	$AgPd_3F_4$_$TlPt_3O_4$_3	357.86	-81.9005
Ag_3Pd_7F_Sm_3MoO_7_2	332.63	-36.8341	$AgPd_{11}F_2$_$NdHf_2F_{11}$_6	357.90	-6.99121
$AgPd_6F$_$EuZrF_6$_1	333.21	-98.002	$Ag_3Pd_9F_2$_$Ba_3Re_2O_9$_2	358.83	-61.0188
Ag_6PdF_$LiWF_6$_3	334.33	-12.983	$AgPd_4F$_$NdBPt_4$_4	359.48	-229.023
Ag_4PdF_$CuTeO_4$_4	334.36	-54.1943	Ag_3Pd_4F_Fe_3NiP_4_6	359.96	-232.559
$Ag_{24}Pd_{11}F_7$_$Li_7Ti_{11}O_{24}$_3	334.47	-9.84313	$Ag_4Pd_{51}F$_$U_4Be_{51}B$_3	360.42	-113.971
$Ag_{15}Pd_{24}F_4$_$Ti_4(Ni_5O_8)_3$_3	334.49	-102.744	$Ag_9Pd_5F_2$_$Eu_2Nb_5O_9$_6	362.48	-146.534
Ag_6Pd_2F_Hf_2BIr_6_4	337.41	-80.8681	$AgPd_4F$_$SmBiO_4$_2	362.51	-8.77675
Ag_2Pd_4F_V_2CoO_4_5	338.61	-119.239	$AgPd_5F$_$LaInNi_5$_3	364.21	-34.9042
$Ag_{16}Pd_8F$_$BaTi_8O_{16}$_5	339.63	-12.0574	Ag_6PdF_$FeNiP_6$_3	364.24	-74.3268
Ag_3PdF_$FeSnO_3$_1	340.39	-53.9318	$Ag_{17}Pd_{20}F_2$_$Ti_{20}H_2N_{17}$_2	364.30	-231.96
$Ag_8Pd_{21}F_8$_$Ba_8Mn_8O_{21}$_1	340.92	-68.8382	$AgPd_4F$_$NaYF_4$_5	364.70	-177.225
Ag_4Pd_6F_Na_6ZnO_4_6	341.36	-72.9668	$AgPd_9F_2$_KPu_2F_9_2	365.71	-79.3631
Ag_3Pd_7F_Lu_3SbO_7_2	341.59	-71.67	$Ag_{15}PdF_3$_Zr_3InF_{15}_1	365.98	-195.694
Ag_4Pd_7F_Sm_4PdO_7_5	341.88	-170.584	Ag_6Pd_2F_Nb_2CdO_6_6	366.99	-7.94657

$Ag_2Pd_3F\_Na_2BiO_3\_5$	367.49	-131.795	$AgPdF_3\_LaAlO_3\_1$	396.26	-66.64
$Ag_{11}Pd_4F\_ZnGa_{11}Co_4\_4$	368.49	-382.134	$Ag_8Pd_{16}F\_BaTi_8O_{16}\_6$	396.27	-78.3506
$Ag_6Pd_3F\_Li_3FeF_6\_2$	369.12	-103.476	$Ag_{15}Pd_7F_2\_Mg_2Ti_7O_{15}\_2$	396.53	-24.1093
$Ag_3Pd_6F_{20}\_Nb_3(Ni_{10}B_3)_2\_1$	370.30	-28.7895	$Ag_2Pd_9F\_KPu_2F_9\_5$	397.53	-19.9239
$AgPd_6F\_GdYCo_6\_3$	371.45	-3.31639	$Ag_2Pd_2F\_Li_2HgO_2\_6$	397.61	-12.1282
$Ag_3Pd_7F\_Na_3CeF_7\_5$	371.82	-181.02	$Ag_6Pd_4F\_Li_6RuN_4\_4$	398.77	-222.155
$Ag_2Pd_{12}F_5\_Lu_5(ReO_6)_2\_5$	373.10	-0.52403	$Ag_{16}Pd_6F\_BaTa_6O_{16}\_5$	402.98	-173.633
$Ag_{35}Pd_{32}F\_FeNi_{35}S_{32}\_1$	373.37	-170.467	$AgPd_4F\_TbGaNi_4\_6$	408.11	-191.984
$AgPd_7F_2\_KIn_2F_7\_1$	373.57	-144.34	$Ag_4PdF_2\_Co_2SnO_4\_5$	408.13	-12.8912
$Ag_2PdF_{12}\_BaAs_2F_{12}\_4$	374.47	-162.083	$AgPd_2F\_LiFeO_2\_4$	410.29	-54.109
$Ag_8Pd_{21}F_2\_Ce_8U_2O_{21}\_2$	374.57	-2.51586	$Ag_3Pd_2F\_LiTi_2N_3\_3$	411.91	-117.992
$AgPd_4F\_TbGaCo_4\_4$	374.68	-176.863	$Ag_5Pd_6F\_Li_5IO_6\_6$	414.58	-1.99746
$Ag_2Pd_{21}F_6\_Cr_{21}(WC_3)_2\_5$	376.09	-76.3873	$AgPd_6F\_CrMoF_6\_6$	414.90	-185.66
$Ag_2Pd_3F\_Li_2HfO_3\_6$	379.26	-165.807	$Ag_8Pd_3F_2\_Mn_3Zn_2O_8\_5$	415.66	-171.917
$AgPd_3F_2\_Nb_3AlC_2\_3$	380.07	-53.3995	$Ag_2Pd_9F_5\_Eu_2Nb_5O_9\_2$	417.71	-165.81
$Ag_4Pd_{12}F_3\_Lu_4Zr_3O_{12}\_1$	380.81	-307.37	$Ag_2Pd_6F\_Lu_2TeO_6\_2$	418.15	-109.885
$Ag_6PdF\_CuPdF_6\_5$	382.12	-9.53014	$Ag_3Pd_2F\_MgTa_2N_3\_1$	422.05	-192.883
$AgPd_2F\_ZrTi_2O\_4$	384.13	-51.7708	$AgPd_{51}F_4\_U_4Be_{51}B\_4$	422.82	-280.243
$Ag_{12}Pd_4F_3\_Mn_{12}Ge_4N_3\_6$	384.15	-234.711	$AgPd_2F_2\_K(FeS)_2\_1$	423.20	-364.093
$Ag_3Pd_6F_2\_Ce_3(TaN_3)_2\_2$	386.54	-81.4639	$Ag_{12}PdF_4\_Np(FeP_3)_4\_3$	423.33	-9.46922
$Ag_{20}Pd_{17}F_2\_Ti_{20}H_2N_{17}\_4$	386.61	-55.184	$Ag_6PdF\_UAgF_6\_6$	424.09	-254.421
$AgPd_3F\_ThTaN_3\_4$	387.39	-38	$Ag_2Pd_4F\_Ga_2FeO_4\_4$	424.42	-147.025
$Ag_{30}Pd_{13}F_5\_Mg_5Ti_{13}O_{30}\_2$	387.72	-341.107	$AgPd_2F\_SrCuO_2\_5$	425.25	-161.422
$AgPd_2F\_ZnMoN_2\_3$	388.68	-82.5641	$Ag_2Pd_3F\_LiTi_2N_3\_1$	426.85	-78.7428
$AgPd_5F\_BaYF_5\_2$	391.16	-29.7264	$Ag_4Pd_6F\_Ca_4PtO_6\_2$	429.22	-159.264
$AgPd_3F\_FeSnO_3\_3$	391.72	-6.96541	$Ag_3Pd_3F\_Na_3AuO_3\_5$	429.73	-83.8889
$AgPd_{10}F\_LaCeNi_{10}\_5$	392.46	-272.918	$Ag_3Pd_2F\_Na_3CuO_2\_5$	430.37	-349.262
$Ag_2PdF\_Ti_2CN\_6$	392.56	-21.787	$AgPd_2F\_GaCuO_2\_6$	431.60	-148.926
$Ag_4Pd_{27}F_2\_Al_{27}(FeNi_2)_2\_1$	393.71	-19.65	$AgPd_4F\_MgTeO_4\_5$	432.22	-61.5227
$Ag_2Pd_3F\_Li_2PtO_3\_6$	394.37	-179.93	$Ag_3Pd_{11}F_3\_Bi_3Ir_3O_{11}\_2$	433.24	-105.807
$Ag_7Pd_3F\_Ho_3SbO_7\_6$	394.66	-216.632	$Ag_3Pd_2F\_TaZn_2N_3\_1$	433.28	-212.914
$Ag_{30}Pd_{104}F_{11}\_Ta_{11}(Co_{52}B_{15})_2\_4$	394.78	-75.6191	$AgPd_{15}F_3\_Zr_3InF_{15}\_3$	434.89	-136.492
$Ag_{32}Pd_{19}F_5\_Zn_5Co_{19}O_{32}\_4$	395.84	-60.6951	$AgPd_3F\_CdPbO_3\_2$	436.48	-248.49

$Ag_4PdF\_LiAgF_4\_5$	436.85	-32.3624	$Ag_6Pd_2F\_Li_2SnF_6\_5$	514.16	-170.225
$Ag_2Pd_2F\_Li_2HgO_2\_5$	437.25	-73.77	$Ag_3Pd_4F\_Ti_4CN_3\_2$	514.97	-170.494
$Ag_6Pd_3F\_Ni(PtO_2)_3\_4$	438.17	-57.6434	$AgPd_3F\_GdInO_3\_2$	522.27	-135.238
$Ag_8PdF\_NiP_8W\_2$	440.52	-119.852	$Ag_2Pd_3F\_Li_2TcO_3\_6$	523.93	-188.016
$AgPd_6F_2\_Ta_2CdO_6\_2$	440.84	-264.266	$AgPd_2F\_LiMoN_2\_4$	532.99	-266.019
$Ag_4Pd_7F\_Li_7SbN_4\_2$	440.87	-1.53978	$AgPd_2F\_LiMoN_2\_3$	538.63	-120.07
$Ag_5Pd_8F\_BaNb_5O_8\_2$	441.70	-188.04	$Ag_3Pd_{12}F_5\_Lu_3Sb_5O_{12}\_2$	565.70	-76.7728
$AgPd_{10}F_3\_GaNi_{10}P_3\_6$	442.77	-19.6493	$AgPd_6F\_FeNiP_6\_1$	573.05	-45.4478
$Ag_5Pd_{12}F_3\_Lu_3Sb_5O_{12}\_5$	444.85	-197.844	$Ag_3Pd_4F\_Na_3UO_4\_5$	576.74	-21.8024
$Ag_7Pd_{19}F\_CeTa_7O_{19}\_5$	444.89	-101.35	$Ag_4Pd_6F\_Li_6RuN_4\_2$	580.01	-169.867
$AgPd_3F\_CeCoSi_3\_1$	445.11	-170.225	$AgPd_2F\_Mo_2CN\_5$	584.86	-169.502
$Ag_5Pd_9F_4\_In_5B_4Ir_9\_5$	445.57	-170.494	$Ag_4Pd_2F\_Mn_2SnO_4\_5$	586.10	-31.0111
$AgPd_4F\_TmAlNi_4\_4$	446.40	-135.238	$Ag_7Pd_3F\_Ta_3O_7F\_4$	588.82	-36.1462
$Ag_6Pd_5F\_Li_5OsO_6\_5$	447.96	-188.016	$AgPd_3F\_CuAgF_3\_5$	590.08	-87.784
$Ag_2Pd_5F_2\_K_2Rh_2O_5\_1$	449.61	-162.501	$Ag_3PdF\_AcTiO_3\_1$	602.63	-22.8747
$AgPdF_2\_CrAuO_2\_2$	452.55	-19.4525	$Ag_3Pd_8F\_Na_3UF_8\_5$	610.73	-209.054
$AgPdF_2\_GaAgO_2\_5$	452.55	-78.7462	$AgPd_8F\_NiP_8W\_4$	617.86	-51.7456
$Ag_3Pd_3F\_Na_3AuO_3\_6$	455.56	-11.2126	$Ag_8Pd_5F\_Co_5NiS_8\_3$	624.94	-30.6302
$AgPd_4F\_TbCuNi_4\_6$	473.46	-33.1727	$AgPd_4F_3\_Ti_4CN_3\_5$	625.29	-61.5528
$Ag_2Pd_4F_3\_Cu_2B_3Ir_4\_2$	474.22	-103.974	$Ag_4Pd_2F\_Li(NiO_2)_2\_1$	634.63	-199.79
$AgPd_{12}F_5\_LaSb_5O_{12}\_2$	482.08	-231.77	$Ag_2Pd_3F\_Li_2RhO_3\_6$	635.41	-258.617
$Ag_4Pd_{12}F_3\_Mn_{12}Ge_4N_3\_5$	485.80	-61.22	$AgPd_3F\_PuTlO_3\_5$	649.39	-39.8305
$AgPd_2F\_ScTaN_2\_2$	486.08	-134.289	$AgPd_3F\_Mn_3SnH\_2$	659.58	-286.947
$Ag_7Pd_4F\_Li_7SbN_4\_4$	487.47	-321.384	$AgPdF_3\_CaH_3Pd\_1$	661.64	-28.4374
$Ag_2Pd_6F_9\_Ho_2(B_2Rh_3)_3\_3$	494.12	-29.1278	$Ag_3Pd_6F\_Ni(PtO_2)_3\_2$	674.15	-108.766
$Ag_6PdF_2\_Li_2SnF_6\_3$	494.93	-255.485	$AgPd_4F\_NaErF_4\_2$	676.76	-25.2155
$Ag_3PdF\_CuAgF_3\_6$	495.53	-234.883	$Ag_4PdF\_SbRhO_4\_1$	677.50	-49.6729
$Ag_4PdF\_CoRhS_4\_5$	495.82	-264.266	$AgPd_{12}F_4\_Np(FeP_3)_4\_1$	679.00	-218.173
$Ag_3Pd_2F\_Li_2TcO_3\_5$	496.17	-1.53978	$AgPd_4F\_CoSi_4Ni\_1$	683.86	-19.098
$AgPd_2F\_ScTaN_2\_5$	498.52	-188.04	$AgPd_4F\_GdYH_4\_1$	688.40	-266.019
$Ag_4PdF\_LiVF_4\_3$	505.65	-19.6493	$Ag_4PdF\_CrMoO_4\_1$	699.87	-120.07
$Ag_{11}Pd_2F\_NdHf_2F_{11}\_3$	507.63	-197.844	$Ag_{12}Pd_4F\_Np(FeP_3)_4\_5$	702.33	-76.7728
$AgPd_6F_2\_Li_2SnF_6\_1$	509.73	-101.35	$AgPd_3F\_Al_3BC\_6$	725.52	-45.4478

$Ag_6Pd_3F\_NaTl_3F_6\_4$	727.28	-21.8024	$Ag_3Pd_7F\_Ta_3O_7F\_2$	775.75	-17.0943
$Ag_2Pd_4F\_Ca(AgO_2)_2\_5$	728.19	-169.867	$Ag_3Pd_4F\_Mg_3NiO_4\_2$	818.59	-88.5688
$Ag_2Pd_7F_2\_Tb_2Pt_2O_7\_6$	733.97	-169.502	$Ag_4Pd_{12}F\_Np(FeP_3)_4\_6$	841.88	-150.9
$Ag_4Pd_3F\_Mg_3NiO_4\_4$	744.94	-31.0111	$AgPd_4F\_SbRhO_4\_3$	853.23	-76.3499
$Ag_5Pd_8F\_Co_5NiS_8\_1$	765.84	-59.1424	$AgPd_4F\_NbMoO_4\_2$	1039.53	-59.1424

Table S4 The CGCNN-2 model predicted 259 potentially stable Ag-Pd-F structures with 149 distinct Ag-Pd-F compositions, including potential stable structures， E_d values from CGCNN-2 model and E_d by DFT. The final number (i.e.,. _3) represent different atomic arrangement of the same substitution template (i.e.,. $BiSb_3F_{20}$) after substituting Ag, Pd, and F atoms.

Composition	DFT-E_d (meV/atom)	CGCNN-E_d (meV/atom)	Composition	DFT-E_d (meV/atom)	CGCNN-E_d (meV/atom)
$AgPd_3F_{20}$_$BiSb_3F_{20}$_3	-22.56	-17.4587	$AgPd_3F_8$_$LiCr_3O_8$_6	42.49	-6.17843
Ag_2PdF_6_La_2WO_6_2	-20.42	-52.3521	$Ag_3Pd_{10}F_{30}$_$Na_3(WO_3)_{10}$_5	42.72	-15.9661
Ag_2PdF_6_Na_2PdF_6_3	-19.78	-19.5577	$AgPd_{11}F_{33}$_$La(WO_3)_{11}$_2	43.08	-40.8212
Ag_2PdF_6_$Ni(IO_3)_2$_1	-17.44	-21.1692	$Ag_5Pd_2F_{12}$_$Y_5U_2O_{12}$_3	43.18	-13.858
$AgPd_2F_{12}$_$CaCr_2F_{12}$_2	-8.53	-32.2214	Ag_2PdF_6_Pr_2WO_6_5	45.32	-3.76616
Ag_3PdF_{20}_$BiSb_3F_{20}$_1	-2.40	-22.7538	$AgPd_7F_{19}$_$PrTa_7O_{19}$_3	46.29	-29.1942
Ag_2PdF_6_Tm_2WO_6_5	19.62	-34.7308	$AgPdF_3$_$LuGaO_3$_2	46.84	-23.734
Ag_4PdF_{10}_ZrU_4O_{10}_2	23.36	-7.31805	Ag_6PdF_{12}_Lu_6WO_{12}_2	47.40	-53.7476
$Ag_4Pd_3F_{12}$_$Lu_4Zr_3O_{12}$_2	24.74	-41.0401	Ag_2PdF_6_$LiCu_2F_6$_2	47.93	-105.261
$Ag_2Pd_2F_7$_$Tm_2Ti_2O_7$_6	26.77	-3.04654	$AgPd_9F_{27}$_$Na(WO_3)_9$_5	48.46	-39.3182
Ag_3PdF_7_Er_3TaO_7_3	27.43	-35.0639	$AgPd_3F_8$_$NaSb_3O_8$_3	48.83	-21.6067
$AgPdF_5$_$VAsO_5$_6	28.22	-87.0575	$Ag_{13}Pd_5F_{30}$_$Mg_5Ti_{13}O_{30}$_6	49.59	-37.5051
$Ag_4Pd_3F_{12}$_$Lu_4Hf_3O_{12}$_3	28.75	-47.0014	$AgPdF_5$_$ZnCuF_5$_1	50.02	-77.3714
Ag_3PdF_7_Sm_3MoO_7_1	29.86	-20.2709	$AgPdF_4$_$LiAgF_4$_4	51.67	-60.4226
$AgPdF_7$_$YPtF_7$_3	31.82	-15.4491	$AgPdF_4$_$LiAgF_4$_2	51.71	-67.6207
Ag_3PdF_8_$NaSb_3O_8$_1	33.79	-58.0066	$Ag_2Pd_4F_{13}$_$Na_2W_4O_{13}$_5	51.75	-0.18872
$Ag_3Pd_2F_{12}$_$Cr_3(FeO_6)_2$_6	33.98	-90.429	Ag_3PdF_8_$TaSb_3O_8$_3	52.11	-40.6428
$AgPdF_4$_$MgTeO_4$_3	34.20	-79.5933	$AgPdF_5$_$MgCuF_5$_3	52.67	-82.3253
$AgPdF_4$_$InSbO_4$_3	35.78	-41.331	Ag_3PdF_8_Ho_3ReO_8_3	53.15	-21.7238
$AgPdF_4$_$InSbO_4$_1	36.03	-40.3551	$AgPd_2F_8$_$Co(ReO_4)_2$_1	53.89	-3.29515
$AgPd_3F_9$_$HoTa_3O_9$_3	36.27	-104.826	Ag_2PdF_6_Sb_2WO_6_5	54.72	-11.9711
Ag_2PdF_5_Na_2VF_5_3	36.97	-28.1482	$AgPdF_4$_$CuTeO_4$_1	57.18	-23.186
$AgPdF_4$_$NbGaO_4$_2	37.22	-44.9046	$Ag_6Pd_8F_{25}$_$Ta_8Pb_6O_{25}$_1	58.84	-1.06352
$Ag_3Pd_2F_{12}$_$Ga_2(MoO_4)_3$_5	38.33	-76.9203	$Ag_7Pd_2F_{15}$_$Mg_2Ti_7O_{15}$_6	64.51	-41.0523
Ag_2PdF_5_Ti_2CoO_5_4	39.27	-33.5468	$AgPdF_4$_$LiVF_4$_2	66.40	-64.014
$Ag_{25}Pd_{11}F_{60}$_$Mg_{11}Ti_{25}O_{60}$_6	39.46	-42.6671	$AgPd_2F_6$_Ta_2CdO_6_1	67.36	-3.62654
$AgPdF_3$_$YMoN_3$_4	41.61	-25.1368	$AgPd_6F_{18}$_$Tl(WO_3)_6$_5	67.74	-10.5765
Ag_3PdF_7_Lu_3SbO_7_1	42.02	-34.3844	$AgPdF_6$_$CuPdF_6$_4	73.59	-105.794

$Ag_2Pd_2F_7$_$Y_2Fe_2O_7$_1	73.95	-47.2514	$Ag_5Pd_3F_{13}$_$Pr_5Ge_3O_{13}$_3	98.72	-3.59357
$Ag_5Pd_2F_{12}$_$Lu_5(ReO_6)_2$_1	74.64	-60.956	$AgPdF_5$_$ZnCuF_5$_3	99.55	-60.5389
Ag_3PdF_9_$Tm(IO_3)_3$_1	75.35	-29.415	$AgPdF_6$_$LiWF_6$_4	99.98	-41.6532
$Ag_2Pd_2F_7$_$Tm_2Ti_2O_7$_5	76.21	-42.6644	$Ag_4Pd_4F_{13}$_$Ru_4Pb_4O_{13}$_1	100.99	-23.4868
$AgPd_{12}F_{33}$_$Ta_{12}MoO_{33}$_3	76.42	-9.19462	Ag_6PdF_{12}_KMn_6O_{12}_4	101.53	-87.4634
$AgPd_4F_8$_$NaTa_4O_8$_3	76.50	-97.214	$Ag_{13}PdF_{33}$_$NaNb_{13}O_{33}$_1	102.44	-46.7701
$Ag_3Pd_2F_{12}$_$Nd_2(MoO_4)_3$_5	78.78	-13.8397	$AgPd_9F_4$_H_9BrO_4_1	102.52	-166.138
$AgPd_2F_6$_Mn_2TeO_6_5	80.01	-42.7866	$AgPdF_6$_$ZrNiF_6$_6	102.74	-63.5626
Ag_3PdF_{12}_Cu_3SbF_{12}_1	81.41	-127.332	$Ag_3Pd_3F_{11}$_$Bi_3Ir_3O_{11}$_1	102.92	-5.96195
$AgPdF_4$_$LiCuF_4$_2	82.17	-69.1169	$Ag_3Pd_{16}F_{32}$_$Sr_3(RhO_2)_{16}$_5	103.22	-24.9151
$AgPdF_6$_$CrNiF_6$_5	82.29	-138.389	$AgPd_{14}F$_$NaAlB_{14}$_6	104.15	-93.9865
$AgPdF_6$_$NaVF_6$_3	83.18	-1.64385	$Ag_{21}Pd_{32}F_3$_$Co_{21}Cu_3O_{32}$_2	105.88	-102.837
$Ag_3Pd_3F_{10}$_$Tl_3Os_3O_{10}$_3	83.53	-8.03935	$AgPdF_4$_$NbGaO_4$_4	106.40	-76.2894
Ag_3PdF_6_Na_3TiF_6_2	83.67	-23.4447	Ag_8PdF_{16}_$BaTi_8O_{16}$_4	107.16	-20.0649
Ag_2PdF_6_Nb_2CdO_6_3	84.08	-32.8894	$AgPdF_4$_$AlSbO_4$_1	107.16	-8.83626
$AgPd_8F_{16}$_$BaTi_8O_{16}$_2	85.26	-35.6304	$AgPdF_5$_$TaAsO_5$_4	107.92	-123.167
Ag_3PdF_6_Li_3NiF_6_6	87.85	-49.9314	Ag_2PdF_7_TiV_2O_7_5	108.10	-3.16804
$AgPdF_4$_$MgTeO_4$_1	88.03	-118.646	$AgPd_2F_5$_$TmMn_2O_5$_5	108.83	-58.8493
$Ag_4Pd_2F_9$_$Ca_4Ta_2O_9$_2	88.32	-4.63566	Ag_3PdF_8_Cr_3AgO_8_6	108.84	-29.8364
$Ag_2Pd_3F_{12}$_$Nd_2(MoO_4)_3$_6	88.91	-35.3713	$Ag_{10}Pd_{16}F$_$Sr(H_8O_5)_2$_4	111.06	-85.3424
$AgPd_2F_6$_Li_2SnF_6_2	89.65	-49.1451	Ag_8PdF_{16}_$BaMn_8O_{16}$_4	111.52	-74.4112
$Ag_5Pd_{13}F_{30}$_$Mg_5Ti_{13}O_{30}$_5	90.14	-6.77787	Ag_2PdF_4_MgV_2O_4_3	111.94	-1.34123
$AgPd_9F_{25}$_Nb_9VO_{25}_3	90.23	-15.0086	$Ag_{20}Pd_3F_{40}$_$Ba_3Ti_{20}O_{40}$_4	114.29	-61.3416
$Ag_2Pd_4F_9$_$Mg_4Sb_2O_9$_1	90.35	-50.793	$Ag_{16}Pd_3F_{32}$_$Rb_3Mn_{16}O_{32}$_6	115.21	-60.242
$Ag_2Pd_4F_{15}$_$Dy_2Mo_4O_{15}$_1	90.72	-4.00677	Ag_8PdF_{16}_$NaMn_8O_{16}$_6	116.40	-166.526
Ag_3PdF_6_Ca_3WO_6_2	90.91	-28.4269	$AgPdF_4$_$AsRhO_4$_2	116.41	-114.19
$AgPdF_7$_$LuPtF_7$_3	91.99	-15.2797	$AgPd_3F_8$_V_3AgO_8_1	116.69	-78.0871
Ag_2PdF_5_Sc_2TiO_5_2	92.38	-16.9269	Ag_7PdF_{19}_$PrTa_7O_{19}$_1	118.48	-107.961
$AgPd_3F_{12}$_Cu_3SbF_{12}_3	93.98	-90.5589	Ag_5PdF_8_$LiAl_5O_8$_2	119.35	-33.1363
Ag_3PdF_6_Pr_3GaO_6_5	94.33	-15.9133	$AgPdF_3$_$TmRhO_3$_5	120.95	-10.9727
$Ag_2Pd_3F_{12}$_$Ga_2(MoO_4)_3$_6	95.52	-33.3508	$Ag_{32}PdF_{35}$_$FeNi_{35}S_{32}$_5	121.09	-1846
$Ag_3Pd_9F_{20}$_$Mg_3Ti_9O_{20}$_5	97.36	-2.49028	Ag_2PdF_6_Li_2SnF_6_4	121.15	-24.4608

$Ag_4Pd_2F_{15}$_$Tm_2Mo_4O_{15}$_1	97.57	-33.0741	$AgPdF_4$_$ZnCrO_4$_4	121.91	-16.475

$Ag_{12}PdF_{33}$_$Ta_{12}MoO_{33}$_1	123.50	-86.2497	Ag_4Pd_9F_H_9BrO_4_6	161.09	-45.0651
$Ag_4Pd_2F_9$_$Mg_4Sb_2O_9$_3	124.70	-91.9513	Ag_7PdF_{10}_$BaGe_7N_{10}$_6	161.15	-51.2542
$Ag_{12}Pd_{19}F$_$EuAl_{12}O_{19}$_5	125.09	-15.9733	$Ag_2Pd_2F_7$_$Sm_2Ge_2O_7$_1	161.19	-8.35988
$AgPdF_4$_$AgRuO_4$_1	129.21	-203.723	$Ag_{16}Pd_3F_{32}$_$Sr_3(RhO_2)_{16}$_6	162.29	-27.1732
Ag_2PdF_5_Ce_2TiO_5_2	129.57	-40.0768	$Ag_{19}Pd_{32}F_5$_$Zn_5Co_{19}O_{32}$_2	163.29	-32.0945
$Ag_2Pd_{28}F$_$Mg(AlB_{14})_2$_3	129.85	-11.5515	$AgPdF_5$_$VAsO_5$_5	164.46	-58.4425
$AgPd_2F_4$_MgV_2O_4_1	131.21	-58.4425	Ag_3PdF_7_Ta_3O_7F_1	164.96	-22.5587
$Ag_3Pd_2F_8$_$Ca_3(AsO_4)_2$_2	132.42	-30.3693	Ag_4PdF_7_$BaGa_4O_7$_4	165.17	-27.0694
$AgPd_3F_6$_Li_3FeF_6_5	132.47	-3.01931	Ag_9PdF_{27}_$Na(WO_3)_9$_6	165.50	-42.425
Ag_9PdF_{25}_Nb_9VO_{25}_1	132.61	-40.0807	Ag_4PdF_8_$NaTa_4O_8$_1	166.25	-30.2707
Ag_6PdF_{12}_$RbMn_6O_{12}$_6	132.75	-64.2628	$Ag_2Pd_{13}F$_$LiB_{13}C_2$_1	168.95	-1.70281
Ag_5PdF_8_Co_5SbO_8_1	133.27	-132.594	Ag_2PdF_4_Fe_2NiO_4_3	169.67	-31.401
Ag_6Pd_2F_Ni_6Ge_2B_4	135.42	-114.802	Ag_3PdF_6_Li_3FeF_6_6	172.48	-6.21313
$Ag_{12}Pd_3F$_$Nb(GaNi_4)_3$_5	136.33	-35.0695	$Ag_4Pd_{12}F$_$Mn_{12}Pt_4N$_5	176.86	-12.0088
Ag_3PdF_{12}_$Er(ReO_4)_3$_1	136.51	-73.4033	$AgPdF_5$_$MgCuF_5$_1	177.30	-18.038
$Ag_2Pd_3F_6$_$Na_2Nb_3O_6$_3	138.85	-5.47458	$Ag_{13}Pd_2F$_$LiB_{13}C_2$_3	179.66	-46.4161
Ag_5PdF_{13}_KSb_5O_{13}_3	139.86	-126.092	$AgPd_3F_7$_Ta_3O_7F_3	182.31	-58.2003
$AgPd_3F_8$_Cr_3AgO_8_5	140.30	-2.26215	$Ag_{35}PdF_{32}$_$FeNi_{35}S_{32}$_2	183.17	-66.223
$Ag_9Pd_3F_{20}$_$Mg_3Ti_9O_{20}$_6	143.40	-26.9374	$Ag_{11}Pd_{17}F$_$KAl_{11}O_{17}$_5	183.58	-10.6893
$Ag_{11}PdF_{33}$_$La(WO_3)_{11}$_4	143.42	-171.101	$Ag_{11}Pd_{25}F_{60}$_$Mg_{11}Ti_{25}O_{60}$_5	187.32	-9.21874
$Ag_{11}PdF_{17}$_$Al_{11}TlO_{17}$_1	143.97	-40.8828	Ag_4PdF_8_$RbMn_4O_8$_6	191.12	-15.3271
Ag_8PdF_{16}_KMn_8O_{16}_4	145.43	-0.71893	Ag_8PdF_5_$BaNb_5O_8$_6	192.58	-17.6489
$Ag_4Pd_2F_3$_$Cu_2B_3Ir_4$_4	145.83	-50.1547	Ag_6PdF_8_$In(Cu_3O_4)_2$_1	192.59	-79.5199
$AgPdF_5$_$TaAsO_5$_2	146.31	-53.6564	$AgPd_2F_4$_$Lu(CuO_2)_2$_3	192.99	-5.64997
$Ag_7Pd_2F_{12}$_$Co_7(SbO_6)_2$_1	149.00	-18.8944	$Ag_{17}Pd_3F_{47}$_$Sm_3Ta_{17}O_{47}$_4	193.75	-37.3272
Ag_3PdF_8_$LiCr_3O_8$_5	151.29	-6.5205	Ag_4PdF_8_Nd_4GeO_8_4	195.49	-22.7998
Ag_2PdF_4_Cd_2PbO_4_1	152.59	-84.4417	Ag_3PdF_8_V_3AgO_8_3	197.82	-1.91845
$Ag_{12}Pd_4F$_$Mn_{12}Pt_4N$_6	152.79	-14.9074	Ag_4PdF_{12}_$K(WO_3)_4$_4	198.74	-16.6504
$AgPdF_3$_$TiVO_3$_5	153.12	-23.7761	$Ag_{27}Pd_7F_9$_$Na_7(WO_3)_9$_1	199.36	-1.98617
Ag_7PdF_{12}_Mn_7GeO_{12}_4	153.17	-56.2466	$Ag_2Pd_{14}F$_$Y_2Fe_{14}C$_5	200.23	-27.6333
$Ag_8Pd_{16}F$_$NaMn_8O_{16}$_4	153.67	-37.352	$Ag_2Pd_2F_{11}$_$Ta_2Mo_2O_{11}$_3	201.92	-14.4389

$AgPd_2F_8$_$CaCu_2F_8$_3	158.14	-111.156	Ag_2PdF_4_$Lu(CuO_2)_2$_1	202.40	-44.1645
$AgPdF_3$_Al_3BC_4	158.83	-119.357	$Ag_3Pd_8F_{12}$_$Al_3(V_3C_2)_4$_3	204.82	-102.26

$Ag_{19}Pd_5F_{32}$_$Zn_5Co_{19}O_{32}$_1	204.93	-4.7357	$Ag_2Pd_2F_7$_$Sm_2Ge_2O_7$_1	161.19	-17.0516
$AgPd_2F_4$_$SrNb_2O_4$_3	205.03	-17.5201	$Ag_{16}Pd_3F_{32}$_$Sr_3(RhO_2)_{16}$_6	162.29	-3.82591
Ag_6PdF_$BaIrF_6$_3	209.12	-2.91891	$Ag_{19}Pd_{32}F_5$_$Zn_5Co_{19}O_{32}$_2	163.29	-37.2218
$Ag_{17}Pd_{11}F$_$KAl_{11}O_{17}$_6	209.27	-14.4557	$AgPdF_5$_$VAsO_5$_5	164.46	-168.525
$AgPd_2F_4$_MgV_2O_4_1	131.21	-17.8073	Ag_3PdF_7_Ta_3O_7F_1	164.96	-234.582
$Ag_3Pd_2F_8$_$Ca_3(AsO_4)_2$_2	132.42	-22.5587	Ag_4PdF_7_$BaGa_4O_7$_4	165.17	-16.3051
$AgPd_3F_6$_Li_3FeF_6_5	132.47	-2.16032	Ag_9PdF_{27}_$Na(WO_3)_9$_6	165.50	-68.7977
Ag_9PdF_{25}_Nb_9VO_{25}_1	132.61	-0.45285	Ag_4PdF_8_$NaTa_4O_8$_1	166.25	-49.0265
Ag_6PdF_{12}_$RbMn_6O_{12}$_6	132.75	-7.56481	$Ag_2Pd_{13}F$_$LiB_{13}C_2$_1	168.95	-135.534
Ag_5PdF_8_Co_5SbO_8_1	133.27	-56.3789	Ag_2PdF_4_Fe_2NiO_4_3	169.67	-3.59357
Ag_6Pd_2F_Ni_6Ge_2B_4	135.42	-2.00282	Ag_3PdF_6_Li_3FeF_6_6	172.48	-60.5389
$Ag_{12}Pd_3F$_$Nb(GaNi_4)_3$_5	136.33	-28.177	$Ag_4Pd_{12}F$_$Mn_{12}Pt_4N$_5	176.86	-41.6532
Ag_3PdF_{12}_$Er(ReO_4)_3$_1	136.51	-0.93376	$AgPdF_5$_$MgCuF_5$_1	177.30	-23.4868
$Ag_2Pd_3F_6$_$Na_2Nb_3O_6$_3	138.85	-32.6544	$Ag_{13}Pd_2F$_$LiB_{13}C_2$_3	179.66	-87.4634
Ag_5PdF_{13}_KSb_5O_{13}_3	139.86	-28.622	$AgPd_3F_7$_Ta_3O_7F_3	182.31	-46.7701
$AgPd_3F_8$_Cr_3AgO_8_5	140.30	-134.084	$Ag_{35}PdF_{32}$_$FeNi_{35}S_{32}$_2	183.17	-166.138
$Ag_9Pd_3F_{20}$_$Mg_3Ti_9O_{20}$_6	143.40	-19.7906	$Ag_{11}Pd_{17}F$_$KAl_{11}O_{17}$_5	183.58	-63.5626
$Ag_{11}PdF_{33}$_$La(WO_3)_{11}$_4	143.42	-5.63189	$Ag_{11}Pd_{25}F_{60}$_$Mg_{11}Ti_{25}O_{60}$_5	187.32	-5.96195
$Ag_{11}PdF_{17}$_$Al_{11}TlO_{17}$_1	143.97	-29.0225	Ag_4PdF_8_$RbMn_4O_8$_6	191.12	-24.9151
Ag_8PdF_{16}_KMn_8O_{16}_4	145.43	-0.46481	Ag_8PdF_5_$BaNb_5O_8$_6	192.58	-93.9865
$Ag_4Pd_2F_3$_$Cu_2B_3Ir_4$_4	145.83	-52.4847	Ag_6PdF_8_$In(Cu_3O_4)_2$_1	192.59	-102.837
$AgPdF_5$_$TaAsO_5$_2	146.31	-7.47947	$AgPd_2F_4$_$Lu(CuO_2)_2$_3	192.99	-76.2894
$Ag_7Pd_2F_{12}$_$Co_7(SbO_6)_2$_1	149.00	-38.2336	$Ag_{17}Pd_3F_{47}$_$Sm_3Ta_{17}O_{47}$_4	193.75	-20.0649
Ag_3PdF_8_$LiCr_3O_8$_5	151.29	-3.372	Ag_4PdF_8_Nd_4GeO_8_4	195.49	-8.83626
Ag_2PdF_4_Cd_2PbO_4_1	152.59	-18.2205	Ag_3PdF_8_V_3AgO_8_3	197.82	-123.167
$Ag_{12}Pd_4F$_$Mn_{12}Pt_4N$_6	152.79	-279.809	Ag_4PdF_{12}_$K(WO_3)_4$_4	198.74	-3.16804
$AgPdF_3$_$TiVO_3$_5	153.12	-43.9928	$Ag_{27}Pd_7F_9$_$Na_7(WO_3)_9$_1	199.36	-58.8493
Ag_7PdF_{12}_Mn_7GeO_{12}_4	153.17	-95.0113	$Ag_2Pd_{14}F$_$Y_2Fe_{14}C$_5	200.23	-29.8364
$Ag_8Pd_{16}F$_$NaMn_8O_{16}$_4	153.67	-4.86381	$Ag_2Pd_2F_{11}$_$Ta_2Mo_2O_{11}$_3	201.92	-85.3424
$AgPd_2F_8$_$CaCu_2F_8$_3	158.14	-0.95292	Ag_2PdF_4_$Lu(CuO_2)_2$_1	202.40	-74.4112

$AgPdF_3\_Al_3BC\_4$	158.83	-18.5255	$Ag_3Pd_8F_{12}\_Al_3(V_3C_2)_4\_3$	204.82	-1.34123
$Ag_4Pd_9F\_H_9BrO_4\_6$	161.09	-34.7279	$Ag_{19}Pd_5F_{32}\_Zn_5Co_{19}O_{32}\_1$	204.93	-61.3416
$Ag_7PdF_{10}\_BaGe_7N_{10}\_6$	161.15	-15.4188	$AgPd_2F_4\_SrNb_2O_4\_3$	205.03	-60.242

$Ag_6PdF\_BaIrF_6\_3$	209.12	-166.526	$Ag_2PdF_4\_Ni(AsO_2)_2\_6$	254.16	-6.5205
$Ag_{17}Pd_{11}F\_KAl_{11}O_{17}\_6$	209.27	-3.59357	$AgPd_{14}F\_NaAlB_{14}\_1$	255.40	-84.4417
$Ag_{19}Pd_5F_{32}\_Mg_5Co_{19}O_{32}\_1$	210.74	-60.5389	$Ag_{19}Pd_{32}F_5\_Mg_5Co_{19}O_{32}\_2$	264.11	-14.9074
$Ag_3PdF_9\_HoTa_3O_9\_1$	211.83	-41.6532	$Ag_{17}Pd_{57}F_{19}\_Na_{17}(WO_3)_{19}\_3$	267.50	-23.7761
$Ag_{57}Pd_{17}F_{19}\_Na_{17}(WO_3)_{19}\_1$	215.57	-23.4868	$Ag_9Pd_4F\_H_9BrO_4\_5$	278.58	-51.2542
$Ag_4PdF_{12}\_ThV_4O_{12}\_1$	215.79	-87.4634	$Ag_{64}Pd_{103}F_7\_Ba_7Al_{64}O_{103}\_5$	283.41	-8.35988
$Ag_{21}Pd_3F_{32}\_Co_{21}Cu_3O_{32}\_1$	216.06	-203.723	$Ag_2PdF_4\_Co(NiO_2)_2\_3$	285.38	-47.2514
$Ag_6PdF_{16}\_BaTa_6O_{16}\_4$	217.49	-40.0768	$Ag_2Pd_2F\_Cr_2Ir_2C\_5$	288.27	-60.956
$Ag_4PdF_6\_Ca_4PtO_6\_1$	217.73	-11.5515	$AgPd_{16}F_{10}\_Ba(H_8O_5)_2\_1$	289.17	-29.415
$Ag_{15}Pd_2F_{32}\_K_2Ta_{15}O_{32}\_3$	218.24	-58.4425	$Ag_{103}Pd_{64}F_7\_Ba_7Al_{64}O_{103}\_6$	292.47	-42.6644
$AgPdF_6\_LiWF_6\_2$	220.04	-30.3693	$AgPd_{16}F_8\_Mn_8PbO_{16}\_1$	293.24	-9.19462
$AgPd_2F_5\_Ti_2CoO_5\_2$	224.50	-3.01931	$Ag_3Pd_2F_6\_Na_2Nb_3O_6\_1$	294.64	-97.214
$AgPdF_3\_ScGaO_3\_4$	227.19	-40.0807	$Ag_{12}PdF_{19}\_EuAl_{12}O_{19}\_3$	295.13	-13.8397
$Ag_2Pd_3F_8\_Ca_2V_3O_8\_1$	228.04	-64.2628	$AgPdF_4\_TlAsO_4\_6$	295.59	-42.7866
$AgPdF_3\_TiFeO_3\_5$	232.93	-132.594	$Ag_6PdF_{18}\_Tl(WO_3)_6\_6$	298.53	-127.332
$AgPd_{13}F_2\_LiB_{13}C_2\_6$	233.40	-114.802	$AgPdF_4\_GdAsO_4\_5$	308.37	-69.1169
$Ag_5PdF_8\_Co_5NiS_8\_2$	234.56	-35.0695	$AgPd_2F\_V_2GaN\_6$	326.67	-138.389
$Ag_2PdF_5\_TmMn_2O_5\_6$	238.09	-73.4033	$Ag_3Pd_{30}F_{10}\_Na_3(WO_3)_{10}\_3$	327.16	-1.64385
$Ag_{64}Pd_7F_{103}\_Ba_7Al_{64}O_{103}\_3$	239.82	-5.47458	$AgPd_2F_4\_Fe_2NiO_4\_1$	340.35	-8.03935
$Ag_4Pd_{17}F_4\_Ni_{17}(GeSe)_4\_2$	240.00	-126.092	$AgPdF_2\_Mo_2CN\_1$	348.65	-23.4447
$Ag_3Pd_5F_{12}\_Sm_3Al_5O_{12}\_1$	240.80	-2.26215	$Ag_2Pd_2F_{11}\_Ta_2Mo_2O_{11}\_1$	353.77	-32.8894
$Ag_5Pd_3F_{12}\_Tm_3Al_5O_{12}\_1$	242.02	-26.9374	$Ag_2PdF_4\_Zn(CuO_2)_2\_3$	356.11	-35.6304
$Ag_2PdF_3\_TaZn_2N_3\_5$	242.11	-171.101	$Ag_2Pd_{21}F_6\_Al_2(Ni_7B_2)_3\_2$	376.31	-49.9314
$Ag_3PdF_6\_Ni(PtO_2)_3\_1$	245.42	-40.8828	$Ag_5Pd_{16}F_7\_Li_5Mn_7O_{16}\_4$	406.53	-118.646
$Ag_7Pd_{27}F_9\_Na_7(WO_3)_9\_3$	245.80	-0.71893	$AgPd_2F_7\_TiV_2O_7\_6$	410.70	-4.63566
$Ag_{16}Pd_{10}F\_Ba(H_8O_5)_2\_5$	246.00	-50.1547	$AgPdF_2\_LiMoN_2\_6$	411.51	-35.3713
$Ag_{19}Pd_{12}F\_EuAl_{12}O_{19}\_6$	246.55	-53.6564	$AgPd_2F\_SrCuO_2\_5$	425.25	-49.1451
$Ag_7PdF_{12}\_Y_7HoO_{12}\_1$	250.03	-18.8944	$Ag_3Pd_{32}F_{21}\_Co_{21}Cu_3O_{32}\_5$	441.43	-6.77787
$Ag_4Pd_{12}F_3\_Mn_{12}Ge_4N_3\_5$	485.80	-15.0086	$Ag_6PdF_{18}\_Rb(WO_3)_6\_6$	275.56	-119.357

$AgPd_3F\_LaAlO_3\_5$	504.54	-50.793	$Ag_2PdF_8\_Co(ReO_4)_2\_3$	277.75	-45.0651
$AgPd_2F_4\_Co(NiO_2)_2\_1$	510.31	-4.00677	$Ag_3PdF\_AcGaO_3\_1$	610.61	-15.2797
$Ag_5Pd_8F\_LiAl_5O_8\_1$	546.45	-28.4269	$AgPd_3F\_CaH_3Pd\_5$	648.44	-16.9269
$Ag_2PdF_8\_CaCu_2F_8\_1$	267.95	-56.2466	$Ag_2Pd_4F\_Be(CoO_2)_2\_5$	1110.23	-90.5589
$AgPd_{28}F_2\_Mg(AlB_{14})_2\_4$	273.23	-37.352	$AgPd_4F_2\_Be(CoO_2)_2\_2$	1437.81	-15.9133
$Ag_2Pd_2F_7\_Sc_2Pt_2O_7\_3$	273.96	-111.156			

	Composition	Symmetry	E_d (meV/atom)
ML+DFT predicted metastable phase (CGCNN-1 and CGCNN-2)	$Ag_3PdF_7\_Er_3TaO_7$	$P\bar{1}$	27.43
	$Ag_4Pd_3F_{12}\_Lu_4Hf_3O_{12}$	$P\bar{1}$	28.75
	$Ag_3PdF_7\_Sm_3MoO_7$	$P2_12_12_1$	29.86
	$Ag_2PdF_5\_Na_2VF_5$	$P2_1/c$	36.97
	$Ag_3Pd_2F_{12}\_Ga_2(MoO_4)_3$	$P2_1/c$	38.33
	$Ag_3Pd_{10}F_{30}\_Na_3(WO_3)_{10}$	$P2/m$	42.72
	$AgPd_{11}F_{33}\_La(WO_3)_{11}$	$P\bar{1}$	43.08
	$AgPd_7F_{19}\_PrTa_7O_{19}$	$P\bar{6}c2$	46.29
	$AgPd_9F_{27}\_Na(WO_3)_9$	$R\bar{3}$	48.46
	$AgPd_3F_8\_NaSb_3O_8$	$P2_1/c$	48.83
	$Ag_2Pd_4F_{13}\_Na_2W_4O_{13}$	$C2/m$	51.75
	$AgPdF_5\_MgCuF_5$	$C2/c$	52.67
	$Ag_3PdF_8\_Ho_3ReO_8$	$P2_1/c$	53.15
	$Ag_6Pd_8F_{25}\_Ta_8Pb_6O_{25}$	$C2$	58.84
	$AgPd_6F_{18}\_Tl(WO_3)_6$	$P6/mmm$	67.77
	$AgPd_{12}F_{33}\_Ta_{12}MoO_{33}$	$C2$	76.42
	$AgPd_4F_8\_NaTa_4O_8$	Cm	76.49
	$Ag_3PdF_{12}\_Cu_3SbF_{12}$	$Im\bar{3}m$	81.41
	$AgPdF_6\_NaVF_6$	$Pnma$	83.18
	$Ag_3Pd_3F_{10}\_Tl_3Os_3O_{10}$	$I4_1/amd$	83.53
	$AgPd_8F_{16}\_BaTi_8O_{16}$	$C2$	85.26
	$Ag_5Pd_{13}F_{30}\_Mg_5Ti_{13}O_{30}$	Pm	90.14
	$AgPd_9F_{25}\_Nb_9VO_{25}$	$I\bar{4}$	90.23
	$Ag_3PdF_6\_Ca_3WO_6$	$R\bar{3}$	90.91
	$AgPd_3F_{12}\_Cu_3SbF_{12}$	$Im\bar{3}m$	93.99
	$Ag_3PdF_6\_Pr_3GaO_6$	$Cmc2_1$	94.33
	$Ag_3Pd_9F_{20}\_Mg_3Ti_9O_{20}$	Cm	97.36
	$AgPdF_5\_ZnCuF_5$	$P2_1/c$	99.55

ML+DFT predicted metastable phase (CGCNN-1)	$AgPd_4F_{10}$_ZrU_4O_{10}	*P1*	10.73
	$AgPdF_5$_$CaCuF_5$	$P2_1/c$	20.11
	$AgPdF_4$_$TbSbO_4$	$P\bar{1}$	28.33
	Ag_6PdF_{12}_La_6WO_{12}	$R\bar{3}$	29.27
	$AgPd_3F_7$_Er_3TaO_7	$P\bar{1}$	29.66
	Ag_3PdF_{15}_$CaAs_3F_{15}$	$P2_12_12_1$	33.99
	$Ag_3Pd_2F_{12}$_$Dy_2(SeO_4)_3$	*Pbcn*	34.36
	Ag_3PdF_7_Er_3SbO_7	$C222_1$	36.22
	$AgPd_4F_{12}$_$K(WO_3)_4$	*P3m1*	37.02
	$Ag_2Pd_2F_7$_$Sm_2Mn_2O_7$	$Fd\bar{3}m$	38.04
	$AgPd_5F_{13}$_$NaSb_5O_{13}$	*Ama2*	42.92
	$Ag_3Pd_2F_{12}$_$Ho_2(SeO_4)_3$	$R\bar{3}c$	43.53
	$AgPd_3F_9$_$Tl(WO_3)_3$	*P6mm*	44.89
	$AgPd_2F_6$_Ta_2PbO_6	*Pnma*	45.49
	$AgPd_2F_6$_$Ga(SiNi_3)_2$	*Pm*	46.16
	$AgPd_3F_9$_$GdTa_3O_9$	$P2_1/m$	46.74
	$Ag_3Pd_2F_{12}$_$Y_2Cr_3O_{12}$	*Fddd*	51.42
	$Ag_2Pd_5F_{12}$_$Lu_5(ReO_6)_2$	*C2/m*	52.14
	$Ag_3Pd_2F_9$_$Pr_3Re_2O_9$	$P\bar{1}$	52.16
	$Ag_3Pd_{17}F_{47}$_$Sm_3Ta_{17}O_{47}$	*P2/m*	54.49
	$Ag_2Pd_2F_7$_$Ta_2Pb_2O_7$	$Cmc2_1$	55.49
	$Ag_3Pd_4F_{13}$_$Nb_4Pb_3O_{13}$	*Pmma*	55.69
	$AgPd_2F_6$_Tm_2TeO_6	$P2_12_12_1$	56.29
	$Ag_4Pd_2F_{15}$_$Dy_2Mo_4O_{15}$	$P2_1/c$	57.85
	$AgPdF_4$_$EuSeO_4$	$P2_1/c$	58.84
	$Ag_4Pd_6F_{19}$_$Ta_6Pb_4O_{19}$	*Imma*	59.61
	$AgPdF_5$_$NbVO_5$	*Pnma*	60.46
	$Ag_3Pd_{14}F_{28}$_$Ba_3(RhO_2)_{14}$	$P\bar{1}$	61.22
	$AgPd_6F_{18}$_$Rb(WO_3)_6$	*Pnnm*	61.46

Table S5 The novel Ag-Pd-F metastable compounds with $E_d < 100\ meV/atom$ using machine-learning (ML), including the Ag-Pd-F structures, along with the space group symmetries and E_d values by the CGCNN-1 and CGCNN-2 model.

ML+DFT predicted metastable phase (CGCNN-1) (continued)	$AgPdF_6\_ZnFeF_6$	$R\bar{3}$	68.01
	$Ag_2PdF_7\_Sr_2AlH_7$	$C2/c$	63.40
	$Ag_3Pd_2F_7\_Tb_2Ti_2O_7$	$P2_1$	68.03
	$Ag_5Pd_4F_{15}\_Sr_5Ta_4O_{15}$	$P\bar{3}c1$	63.94
	$AgPd_2F_{12}\_CaAs_2F_{12}$	$P\bar{4}m2$	68.46
	$AgPd_6F_{16}\_BaTa_6O_{16}$	$Amm2$	64.62
	$AgPd_6F_{12}\_Lu_6TeO_{12}$	$R\bar{3}$	69.19
	$Ag_3Pd_4F_{12}\_Lu_4Hf_3O_{12}$	$P\bar{1}$	65.56
	$AgPd_3F_8\_Ho_3ReO_8$	$P2_1/c$	69.53
	$Ag_4Pd_3F\_Ti_4CN_3$	$R3m$	66.43
	$Ag_5Pd_5F_{16}\_La_5Mn_5O_{16}$	$P1$	69.73
	$Ag_7Pd_9F_{27}\_Na_7(WO_3)_9$	$P1$	69.88
	$AgPdF_6\_LiFeF_6$	$P4_2nm$	71.39
	$Ag_5Pd_2F_{12}\_Tb_5(RuO_6)_2$	$C2/m$	72.44
	$Ag_4Pd_3F_{12}\_Mn_{12}Ge_4N_3$	$P4/m$	74.88
	$Ag_4Pd_2F_9\_Sr_4Ru_2O_9$	$P321$	77.44
	$AgPdF_4\_NaYF_4$	$P1$	82.55
	$Ag_{14}Pd_{10}F_{39}\_Nb_{10}Pb_{14}O_{39}$	$Amm2$	84.03
	$Ag_3Pd_5F_{12}\_La_3Sb_5O_{12}$	$I\bar{4}3m$	86.43
	$Ag_{21}Pd_{14}F_{47}\_Sr_{21}Fe_{14}O_{47}$	$P\bar{1}$	86.51
	$AgPd_2F_6\_Tm_2WO_6$	$P2/c$	90.34
	$AgPdF_6\_LiMnF_6$	$R\bar{3}$	90.48
	$AgPdF_3\_YReN_3$	$Pnma$	90.49
	$Ag_8Pd_3F\_Ti_8Cu_3Ni$	$P4/mmm$	90.57
	$AgPd_2F_{12}\_BaAs_2F_{12}$	$Pm\bar{3}m$	92.35
	$AgPd_{13}F_{33}\_NaNb_{13}O_{33}$	$P1$	93.03
	$Ag_3Pd_{16}F_{32}\_Rb_3Mn_{16}O_{32}$	$P\bar{1}$	93.68
	$Ag_2PdF_{12}\_CaCr_2F_{12}$	$P\bar{1}$	94.03
	$AgPd_2F_6\_Hg(SbO_3)_2$	$P\bar{3}1m$	94.76
	$AgPd_6F_{12}\_Rb(IrO_2)_6$	$I4/m$	94.79
	$Ag_{12}Pd_8F_3\_Al_3(V_3C_2)_4$	$P6_3/mcm$	95.68
	$Ag_2Pd_8F_{19}\_U_8Bi_2O_{19}$	$P1$	98.37
	$AgPdF_4\_EuSeO_4$	$P2_1/c$	99.37

ML+DFT predicted metastable phase (CGCNN-2)	$AgPdF_7\_YPtF_7$	$P2_1/c$	31.82
	$Ag_{12}Pd_8F_{27}\_Sr_{12}Fe_8O_{27}$	$P\bar{1}$	99.46
	$Ag_3PdF_8\_NaSb_3O_8$	$P2_1/c$	33.79
	$Ag_2PdF_6\_Tm_2WO_6$	$P2/c$	19.62
	$Ag_3Pd_2F_{12}\_Cr_3(FeO_6)_2$	$P2_1/c$	33.98
	$Ag_4PdF_{10}\_ZrU_4O_{10}$	$P1$	23.36
	$AgPdF_4\_MgTeO_4$	$P2/c$	34.20
	$Ag_4Pd_3F_{12}\_Lu_4Zr_3O_{12}$	$P\bar{1}$	24.74
	$AgPdF_4\_InSbO_4\_1$	$P2_1/c$	35.78
	$Ag_2Pd_2F_7\_Tm_2Ti_2O_7$	$P2_1$	26.77
	$AgPdF_4\_InSbO_4\_2$	$P2_1/c$	36.03
	$AgPdF_5\_VAsO_5$	$Pnma$	28.23
	$AgPd_3F_9\_HoTa_3O_9$	$P2_1/m$	36.27
	$AgPdF_4\_NbGaO_4$	$C2/m$	37.22
	$Ag_2PdF_5\_Ti_2CoO_5$	$Cmcm$	39.27
	$Ag_{25}Pd_{11}F_{60}\_Mg_{11}Ti_{25}O_{60}$	$P1$	39.46
	$AgPdF_3\_YMoN_3$	$C2/c$	41.62
	$Ag_3PdF_7\_Lu_3SbO_7$	$C222_1$	42.02
	$AgPd_3F_8\_LiCr_3O_8$	$Pnnm$	42.49
	$Ag_5Pd_2F_{12}\_Y_5U_2O_{12}$	$P1$	43.18
	$Ag_2PdF_6\_Pr_2WO_6$	$C2/c$	45.32
	$AgPdF_3\_LuGaO_3$	$P6_3cm$	46.84
ML+DFT predicted metastable phase (CGCNN-2) (continued)	$Ag_6PdF_{12}\_Lu_6WO_{12}$	$R\bar{3}$	47.39
	$Ag_2PdF_6\_LiCu_2F_6$	$P4_2/mnm$	47.93
	$Ag_{13}Pd_5F_{30}\_Mg_5Ti_{13}O_{30}$	Pm	49.59
	$AgPdF_5\_ZnCuF_5$	$P2_1/c$	50.02
	$AgPdF_4\_LiAgF_4\_1$	$C2/c$	51.67
	$AgPdF_4\_LiAgF_4\_2$	$C2/c$	51.71
	$Ag_3PdF_8\_TaSb_3O_8$	Pc	52.11
	$AgPd_2F_8\_Co(ReO_4)_2$	$P\bar{3}m1$	53.89
	$Ag_2PdF_6\_Sb_2WO_6$	$P2_1$	54.72
	$AgPdF_4\_CuTeO_4$	$Cmmm$	57.18
	$Ag_7Pd_2F_{15}\_Mg_2Ti_7O_{15}$	$P2_1/m$	64.51

ML+DFT predicted metastable phase (CGCNN-2) (continued)	$Ag_3Pd_2F_{12}\_Nd_2(MoO_4)_3$	*C2/c*	78.78
	$AgPdF_4\_LiVF_4$	$P2_1/c$	66.40
	$AgPd_2F_6\_Mn_2TeO_6$	$P4_2/mnm$	80.01
	$AgPd_2F_6\_Ta_2CdO_6$	*Pbcn*	67.36
	$AgPdF_4\_LiCuF_4$	$P2_1/c$	82.17
	$AgPdF_6\_CuPdF_6$	$P\bar{1}$	73.59
	$AgPdF_6\_CrNiF_6$	$R\bar{3}$	82.29
	$Ag_2Pd_2F_7\_Y_2Fe_2O_7$	$Fd\bar{3}m$	73.95
	$Ag_3PdF_6\_Na_3TiF_6$	$P2_1/c$	83.67
	$Ag_5Pd_2F_{12}\_Lu_5(ReO_6)_2$	*C2/m*	74.64
	$Ag_2PdF_6\_Nb_2CdO_6$	*Pbcn*	84.08
	$Ag_3PdF_9\_Tm(IO_3)_3$	$P2_1/c$	75.35
	$Ag_3PdF_6\_Li_3NiF_6$	$Pnq2_1$	87.85
	$Ag_2Pd_2F_7\_Tm_2Ti_2O_7$	$P2_1$	76.21
	$AgPdF_4\_MgTeO_4$	*P2/c*	88.03
	$Ag_4Pd_2F_9\_Ca_4Ta_2O_9$	$P2_1/c$	88.32
	$Ag_2Pd_3F_{12}\_Nd_2(MoO_4)_3$	*C2/c*	88.91
	$AgPd_2F_6\_Li_2SnF_6$	$P\bar{3}1m$	89.66
	$Ag_2Pd_4F_9\_Mg_4Sb_2O_9$	$P\bar{1}$	90.35
	$Ag_2Pd_4F_{15}\_Dy_2Mo_4O_{15}$	$P2_1/c$	90.72
	$AgPdF_7\_LuPtF_7$	$P2_1/c$	91.99
	$Ag_2PdF_5\_Sc_2TiO_5$	$Cmc2_1$	92.38
	$Ag_2Pd_3F_{12}\_Ga_2(MoO_4)_3$	$P2_1/c$	95.52
	$Ag_4Pd_2F_{15}\_Tm_2Mo_4O_{15}$	$P2_1/c$	97.57
	$Ag_5Pd_3F_{13}\_Pr_5Ge_3O_{13}$	$P6_3/m$	98.72
	$AgPdF_6\_LiWF_6$	$P2_1/c$	99.98

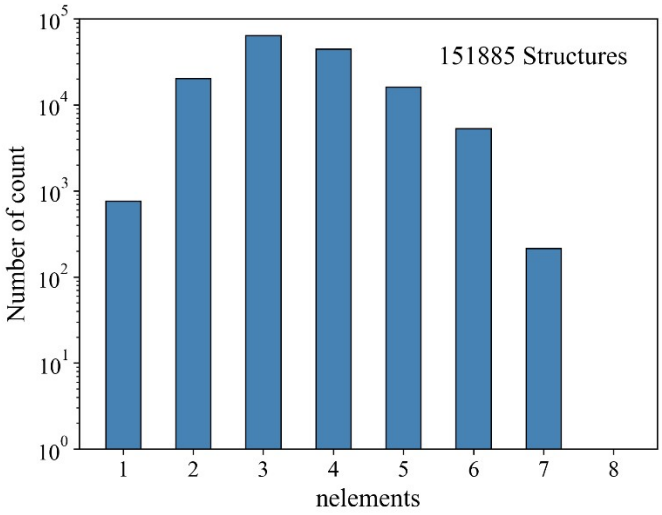

Fig S1 Histogram representing the distribution of the number of elements in each crystal in the training dataset

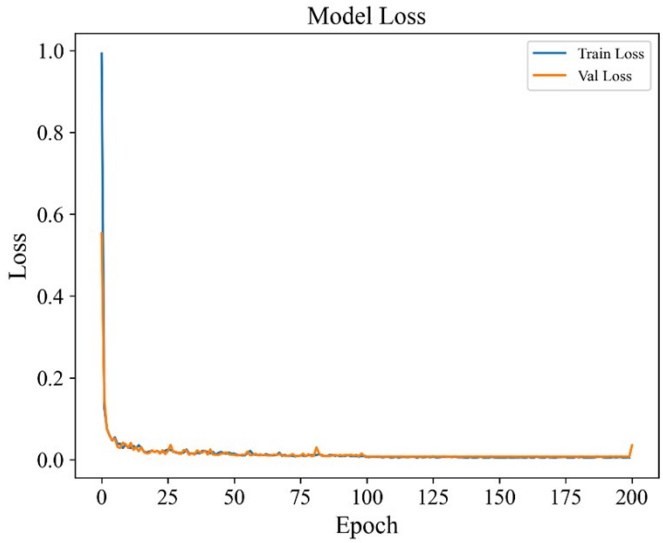

Fig S2 Loss curves of CGCNN model training set and validation set

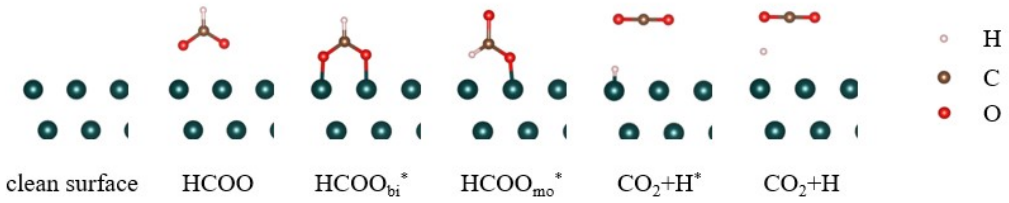

Fig S3 Direct dissociation path for the formate oxidation reaction. $HCOO^-$ initially forms $HCOO_{bi}^{*-}$ on a clean catalyst surface. Then $HCOO_{bi}^{*-}$ transitions to a $HCOO_{mo}^{*-}$, which is more favorable for the reaction. Subsequently, the C-H bond in $HCOO_{mo}^{*-}$ breaks, resulting in the formation of an H^* and CO_2. Ultimately, the reaction products are H and CO_2, with the release of two electrons.The atoms of H, C, and O are represented by white, brown, and red spheres, respectively.

Element replacement and lattice scaling codes

```
import os

import csv

from itertools import permutations

from pymatgen.core import Structure

from pymatgen.transformations.standard_transformations

import SubstitutionTransformation


original_folder_path = "  "

new_folder_path = "  "

csv_file_path = "  "


file_list = [f for f in os.listdir(original_folder_path) if f.endswith(".cif")]  # Get the list of all files ending with ".cif" in the folder

os.makedirs(new_folder_path, exist_ok=True)  # Create the folder to save the new crystal structures

structure_info = []  # Create an empty list to save the new CIF file names and their chemical formulas


# Loop over scaling factors from 0.96 to 1.04 in intervals of 0.02

scaling_factors = [round(x, 2) for x in list((i / 100) for i in range(96, 105, 2))]


# Iterate over each original crystal structure file

for scale_factor in scaling_factors:

    for file_name in file_list:

        file_path = os.path.join(original_folder_path, file_name)  # Build the full path of the original crystal structure file

        structure = Structure.from_file(file_path)  # Read the original crystal structure file

        original_formula = structure.composition.reduced_formula  # Get the chemical formula of the crystal structure


        scaled_structure = structure.copy()

        scaled_structure.scale_lattice(scale_factor)
```

```
        elements = list(set([site.species_string for site in structure.sites]))  # Get all the element types in the crystal structure and determine the order to replace with Ag, Pd, and F

        replacements = ["Ag", "Pd", "F"]

        substitution_mapping = {elements[i]: replacements[i] for i in range(len(elements))}  # Create the substitution mapping dictionary

        unique_permutations = list(permutations(replacements))  # Generate all unique permutations



        # Iterate over all permutations

        for i, perm in enumerate(unique_permutations, start=1):

            permutation_mapping = {elements[i]: perm[i] for i in range(len(elements))}  # Create the substitution mapping dictionary

            substitution = SubstitutionTransformation(permutation_mapping)  # Create substitution transformation object

            new_structure = substitution.apply_transformation(structure)  # Apply substitution transformation and get the substituted crystal structure

            new_formula = new_structure.composition.reduced_formula  # Get the chemical formula of the substituted crystal structure

            # Build the new file path

            new_file_name = f"{new_formula}_{original_formula}_{scale_factor}_{i}.cif"

            new_file_path = os.path.join(new_folder_path, new_file_name)

            new_structure.to(filename=new_file_path)  # Write the substituted crystal structure to the new file

            structure_info.append([new_file_name, original_formula])  # Add the new CIF file name and its chemical formula to the list



# Save the new CIF file names and chemical formulas to a CSV file

with open(csv_file_path, 'w', newline='') as csvfile:

    writer = csv.writer(csvfile)

    for info in structure_info:

        new_formula = info[1].replace("Ag", "Ag").replace("Pd", "Pd").replace("F", "F")  # Replace the chemical formula elements with the "AgPdF" formula

        writer.writerow([info[0], "1"])  # Replace the second column with "1"
```

The POSCAR file for Ag_2PdF_6_La_2WO_6

Ag8 Pd4 F24

1.00000000000000

-5.2378656646866135 -0.0000110436408460 0.0000112985289491

-0.0000287512389392 9.7893631527383835 0.0000370723342309

-0.0000615893699187 0.0000516225476188 -11.2539799866115651

Ag Pd F

8 4 24

Direct

0.0210276948064976 0.3541515448307102 0.9063550707234547

0.9933391141111467 0.3132991069525377 0.3499592522214058

0.5066600741578757 0.6867013833799870 0.8499593642681331

0.4789728563689560 0.6458494874134036 0.4063555472681889

0.5210253123649542 0.1458529303343816 0.0936435220045648

0.4933361838415096 0.1866987474585610 0.6500380069201315

0.0066642049726911 0.8133015115784407 0.1500384188629528

0.9789701348817923 0.8541470569139274 0.5936443437647605

0.9992126486503063 0.9972284128486593 0.8714158578344834

0.5007858850602820 0.0027719048739357 0.3714159466372048

0.4992119759481211 0.5027745458144153 0.1285844743413537

0.0007893215618612 0.4972254971261832 0.6285843492440309

0.7843953602463106 0.6358242163913852 0.5501372282322413

0.8023773683065483 0.5193982025084817 0.7769587957408408

0.7801311362260482 0.8619104141434002 0.7881422430315372

0.7216172344799858 0.8491427845355177 0.3219809915416071

0.7815981975108416 0.3473844894155113 0.5717766816826811

0.8059820184646982 0.9760844330430548 0.0211653699587062

0.6940164678939225 0.0239159308911794 0.5211646702755572

0.7184041375547962 0.6526151910796893 0.0717760631896200

0.7783827912084504 0.1508573320980829 0.8219806307455629

0.7198687833564018 0.1380891308059745 0.2881411205180205

0.6976221844994970 0.4806018173170884 0.2769587625610739

0.7156049166796844 0.3641750382577334 0.0501373740480952

0.2843962078807286 0.8641693962766714 0.4498615040633814

0.3023779225932055 0.9806018288298423 0.2230411712905732

0.2801284428174309 0.6380908001376062 0.2118598124393919

0.2216201208026338 0.6508567312994613 0.6780178951684602

0.2815922438828725 0.1526106538249576 0.4282272568532445

0.3059792475047459 0.5239201194023489 0.9788366679620950

0.1940226226139628 0.4760795443040267 0.4788361392393651

0.2184061660134485 0.8473901241085930 0.9282276434982150

0.2783809409278883 0.3491432326975515 0.1780180428718557

0.2198733426530572 0.3619097637551988 0.7118595070088385

0.1976226654321954 0.0193982369502859 0.7230412538168789

0.2156020937248508 0.1358314884007834 0.9498600101711682

.

The POSCAR file for Ag_2PdF_6_Na_2PdF_6

Ag6 Pd3 F18

1.00000000000000

-0.0000093409817735 0.0000163519957456 -5.1851794796105093

-4.9012816010619877 -8.4893623608309543 -0.0000187777653804

-4.9013072414303922 8.4893563452364038 0.0000345946164288

Ag Pd F

6 3 18

Direct

0.0000000484423452 0.0000004737649988 0.6299186148559962

0.5000008590292211 0.9999992746823381 0.2960225469528441

0.0000000973574359 0.6299190836888621 0.0000000384184773

0.5000001342375526 0.7039756602249594 0.7039749270154485

0.4999990850130231 0.2960232191240836 0.9999985219627376

0.9999998862188306 0.3700819815281441 0.3700815472896714

0.4967394126148739 0.6666668534651450 0.3333329416476190

0.0000002271203314 0.0000002355390905 0.9999997944022141

0.5032603246464242 0.3333334832201587 0.6666662834309918

0.2089371618571508 0.9084489148215861 0.8051598761027017

0.7106693644365433 0.7844848096902032 0.5244788629739664

0.2827135812390831 0.8578081956722574 0.4053253962505495

0.2827137351403659 0.5946751299563047 0.4524815371925456

0.7106690110533503 0.7399947457607012 0.2155158605426117

0.2089365319145318 0.8967107737576818 0.0915497349219737

0.7910619581255034 0.8051604455072501 0.9084485475466645

0.7106694309387177 0.4755211330921991 0.2600043238088179

0.2827131943570971 0.5475174268622652 0.1421919846972611

0.2089385292660143 0.1948400898454049 0.1032896373105251

0.2893304022119643 0.5244794146035138 0.7844839592468892

0.7172858480652770 0.4053260399202430 0.8578073192096571

0.7172863598657634 0.4524822809241996 0.5946746790845523

0.2893309010056604 0.2155160569110230 0.7399938805486215

0.7910637209145364 0.0915510732549665 0.8967112374130715

0.2893308000032184 0.2600045521838115 0.4755205762298952

0.7172871187138802 0.1421921785737919 0.5475168914832352

0.7910632962112771 0.1032901334247859 0.1948397694604632

The POSCAR file for $AgPd_2F_{12}$_$CaCr_2F_{12}$

Ag1 Pd2 F12

1.00000000000000

-1.7720184519496809 -4.3521995859564724 2.2559442904223692

0.0496795107017304 0.0395522959333229 5.5156942684974535

-7.2179952719352558 4.1498485197443280 2.3367316492112189

Ag Pd F

1 2 12

Direct

0.7500000000000000 0.5000000000000000 0.2500000000000000

0.9910378949227806 0.0073842582690488 0.9970564324954280

0.5089621050772123 0.9926157417309514 0.5029435675045720

0.7325410937633768 0.2378166621104323 0.8087927521431592

0.2562322979323836 0.2261890774441783 0.3044455708003296

0.1794120715815921 0.2356408760101130 0.9565284740740453

0.7177481988294325 0.2261231379185604 0.4640819524227793

0.2311158758134728 0.7713109526937756 0.8852883725046681

0.7769993319240129 0.7612093120221207 0.3809852005276472

0.3205879284183654 0.7643591239898441 0.5434715259259547

0.7822518011705675 0.7738768620816667 0.0359180475772705

0.7674589062366232 0.7621833378896031 0.6912072478568408

0.2437677020676163 0.7738109225557012 0.1955544291997061

0.2688841241864702 0.2286890473061393 0.6147116274953319

0.7230006680759871 0.2387906879776655 0.1190147994724169

The POSCAR file for Ag_2PdF_6_Sm_2WO_6

Ag8 Pd4 F24

1.00000000000000

-5.6813877471091638 -0.0000000233834993 0.0000001485219523

0.0000000039921818 -8.0150706979097510 -1.0336843939654468

-0.0000003324699368 -1.6493023765156352 12.7885127800194969

Ag Pd F

8 4 24

Direct

0.2104946464862589 0.0000000327487797 0.7500000206055546

0.7895053535137838 0.9999999672512203 0.2499999793944454

0.7500000487127636 0.2500000154653534 0.5964268561407552

0.2499998936100312 0.2500000422928039 0.0964268557438318

0.2895052681257173 0.5000000317615516 0.7499999792327046

0.7104947318741263 0.4999999682384484 0.2500000207672954

0.7500001063898054 0.7499999577071321 0.9035731442562037

0.2499999512870730 0.7499999845345826 0.4035731438592376

0.7499998343785066 0.2499999810651303 0.8703891880577159

0.2500001068180850 0.2499999824657664 0.3703891875065054

0.7499998931817871 0.7500000175344113 0.6296108124934947

0.2500001656213655 0.7500000189350473 0.1296108119422555

0.8836899692561944 0.0242343203102675 0.8697479185591979

0.5225774976079561 0.1880233551492224 0.9765943352743155

0.1163099295080073 0.0242343041962738 0.3697478977789491

0.5189593302386883 0.1967008045500133 0.7572444998357949

0.4774222461082602 0.1880233534593173 0.4765943985512018

0.9810406578803763 0.3032992826620375 0.7572446411872374

0.4810407482183678 0.1967007988100999 0.2572445467487893

0.0225780630456014 0.3119764951627432 0.4765944915700424

0.6163096975818774 0.4757656790736066 0.8697479573968456

0.0189594224509562 0.3032992753964325 0.2572445944786734

0.6163098012278936 0.5242343377885955 0.6302520230719191

0.0225783209642443 0.6880235025927944 0.0234054441883039

0.9774216790358340 0.3119764974069569 0.9765945558116745

0.3836901987720495 0.4757656622114398 0.3697479769281234

0.9810405775489228 0.6967007246035252 0.7427554055213054

0.3836903024180657 0.5242343209264287 0.1302520426031545

0.9774219369544769 0.6880235048370081 0.5234055084299721

0.5189592517817248 0.8032992011899424 0.7427554532510757

0.0189593421195027 0.6967007173379202 0.2427553588127697

0.5225777538916828 0.8119766465407395 0.5234056014486778

0.4810406697614042 0.8032991954500289 0.2427555001642264

0.8836900704919999 0.9757656958037192 0.6302521022211289

0.4774225023919869 0.8119766448508344 0.0234056647257411

0.1163100307438128 0.9757656796897255 0.1302520814408520

The POSCAR file for $AgPd_2F_6$_Ca_2H_6Os

Ag1 Pd2 F6

1.00000000000000

1.6125945778894279 4.5611062453211790 2.7930957409145463

1.6125945778894282 4.5611062453211790 -2.7930957409145445

-3.2251891557788555 4.5611062453211790 0.0000000000000010

Ag Pd F

1 2 6

Direct

-0.0000000000000000 0.0000000000000000 0.0000000000000000

0.7500000000000000 0.7500000000000000 0.7500000000000000

0.2500000000000000 0.2500000000000000 0.2500000000000000

0.2563756081384901 0.7436243918615029 0.2563756081384901

0.7436243918615029 0.2563756081384901 0.7436243918615029

0.2563756081384901 0.7436243918615029 0.7436243918615029

0.7436243918615029 0.2563756081384901 0.2563756081384901

0.2563756081384901 0.2563756081384901 0.7436243918615029

0.7436243918615029 0.7436243918615029 0.2563756081384901

The POSCAR file for Ag_2PdF_6_$Ni(IO_3)_2$

Ag4 Pd2 F12

1.00000000000000

5.0923456192213159 0.0000023179662980 -0.0000214378373468

0.0000074342592307 -0.0114124609920041 5.6857437843181993

-0.0000047181289273 -9.9210114288343103 -0.0203194566863506

Ag Pd F

4 2 12

Direct

0.4375285608754582 0.2499659682559467 0.0545466256108552

0.9375278046158485 0.7500341010239667 0.9454536659389122

0.9374812188253657 0.2499897398846777 0.3914343924395914

0.4374805471993684 0.7500096425405521 0.6085653716085355

0.4374290861970490 0.7499632457404780 0.2575988114776799

0.9374288033183471 0.2500363679176832 0.7424013339212621

0.2215687814547414 0.6057404233846272 0.1134888972764154

0.7215691381101114 0.3942585929338989 0.8865108825263843

0.2250527828442566 0.6043081768991687 0.4009433365042903

0.7250524274871333 0.3956910654871048 0.5990565660199821

0.6543040873127292 0.4607629838680579 0.2505998999618007

0.1543035166262977 0.5392367733853550 0.7494002327595958

0.1498242125622166 0.1043126134722466 0.5990832083461936

0.6498253772757335 0.8956873514001554 0.4009173999752494

0.2205503044301243 0.0391609485037472 0.2505718333160418

0.7205502497264412 0.9608388680568564 0.7494281068193192

0.1532612827492348 0.1058917570920989 0.8865419821184836

0.6532613083895177 0.8941083901533881 0.1134584683794167

The POSCAR file for Ag_3PdF_{20}_$BiSb_3F_{20}$

Ag3 Pd1 F20

1.00000000000000

0.1705107276830486 0.2557273200695028 -6.2019557109424674

-3.1311273942373550 7.8300336828971018 0.5876883094009085

8.4320200563841237 0.1200999707853954 0.5876883094009049

Ag Pd F

3 1 20

Direct

-0.0000000000000000 0.8001193278967861 0.1998806721032138

0.7890738194496250 0.2138026549708407 0.2131109325237569

0.2109261805503680 0.7868890674762434 0.7861973450291594

-0.0000000000000000 0.1991814883120342 0.8008185116879588

0.7711607645618229 0.4490215867965235 0.2536776953380687

0.7774021001837106 0.2580176962095074 0.4502287692098691

0.2225978998162897 0.5497712307901451 0.7419823037904930

0.2288392354381699 0.7463223046619313 0.5509784132034765

0.0973676671936414 0.2397678484158340 0.2336466762241600

0.9026323328063515 0.7663533237758400 0.7602321515841658

0.8082345787521873 0.3463171198460573 0.7574134358795396

0.7996445307576918 0.7501565227063650 0.3424292034244084

0.2003554692423010 0.6575707965755987 0.2498434772936422

0.1917654212478128 0.2425865641204606 0.6536828801539432

0.7874480731607164 0.1531960706932752 0.9528519919690829

0.7869980032876955 0.9531801416047246 0.1516309885044222

0.2130019967123045 0.8483690114955778 0.0468198583952753

0.2125519268392840 0.0471480080309240 0.8468039293067180

0.4820750428415368 0.1780400461804444 0.1827445947991539

0.5179249571584490 0.8172554052008391 0.8219599538195559

0.1414217078159928 0.3728025765239111 0.9840903426629728

0.1380778138668648 0.9882842508597568 0.3800617104806582

0.8619221861331424 0.6199382895193419 0.0117157491402502

0.8585782921840073 0.0159096573370273 0.6271974234760886

The POSCAR file for $AgPd_3F_{20}$_$BiSb_3F_{20}$

Ag1 Pd3 F20

1.00000000000000

0.0143043159684870 0.0214532213764780 -5.3967988433449365

-3.4658150010203870 8.0463710744150099 0.7027396784254922

8.7604105192487420 -0.1056817047386916 0.7027396784254634

Ag Pd F

1 3 20

Direct

0.0000000000000000 0.1848018296611400 0.8151981703388388

-0.0000000000000000 0.8086350102413929 0.1913649897586071

0.7867680950385331 0.2472555647535515 0.2411697475827965

0.2132319049614670 0.7588302524171823 0.7527444352464273

0.6508993479298635 0.4369820005738691 0.2453834377950451

0.7489143027711649 0.3063655018601829 0.4655699554636076

0.2510856972288065 0.5344300445363993 0.6936344981398382

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