

Supplementary Material

(LaCrO₃)_m/SrCrO₃ superlattices as transparent p-type semiconductors with finite magnetization

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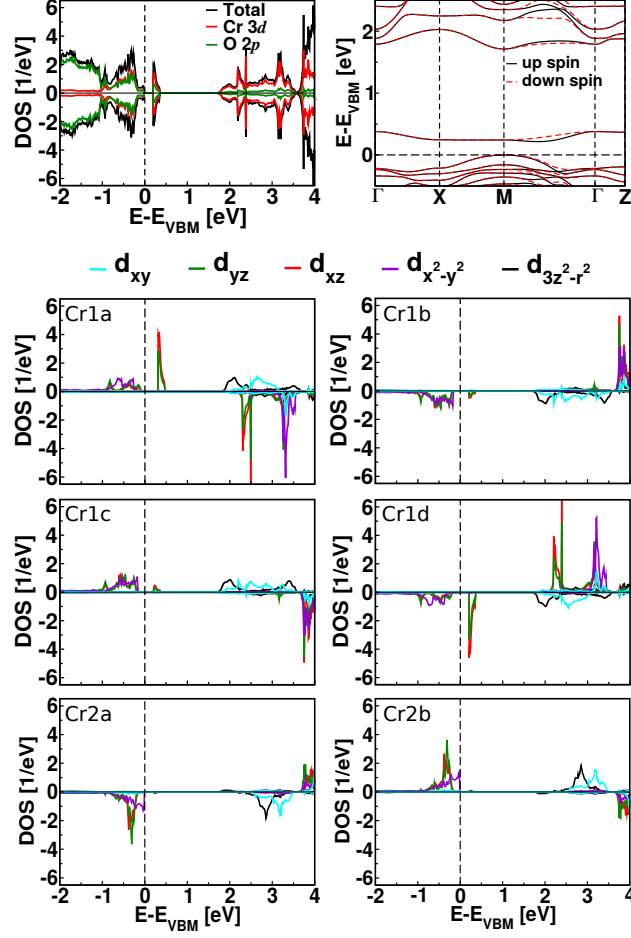


FIG. S1. Total and partial densities of states (sum over all atoms, divided by the number of Cr atoms) as well as band structure of the $m = 2$ superlattice, along with orbitally projected densities of states of the Cr atoms in layers L1 and L2. The labels of the atoms are indicated in Figure 3.

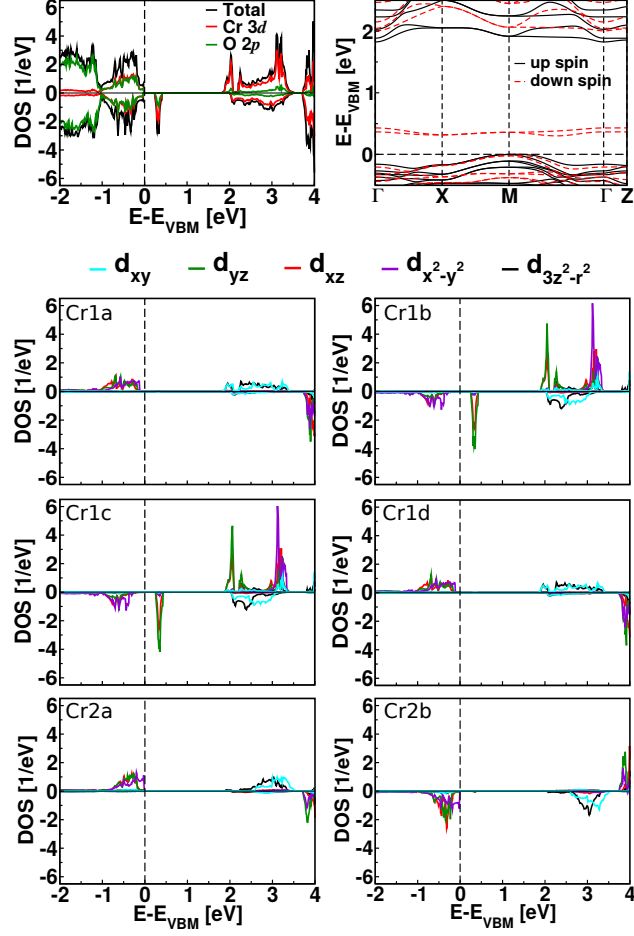


FIG. S2. Total and partial densities of states (sum over all atoms, divided by the number of Cr atoms) as well as band structure of the $m = 3$ superlattice, along with orbitally projected densities of states of the Cr atoms in layers L1 and L2. The labels of the atoms are indicated in Figure 3.

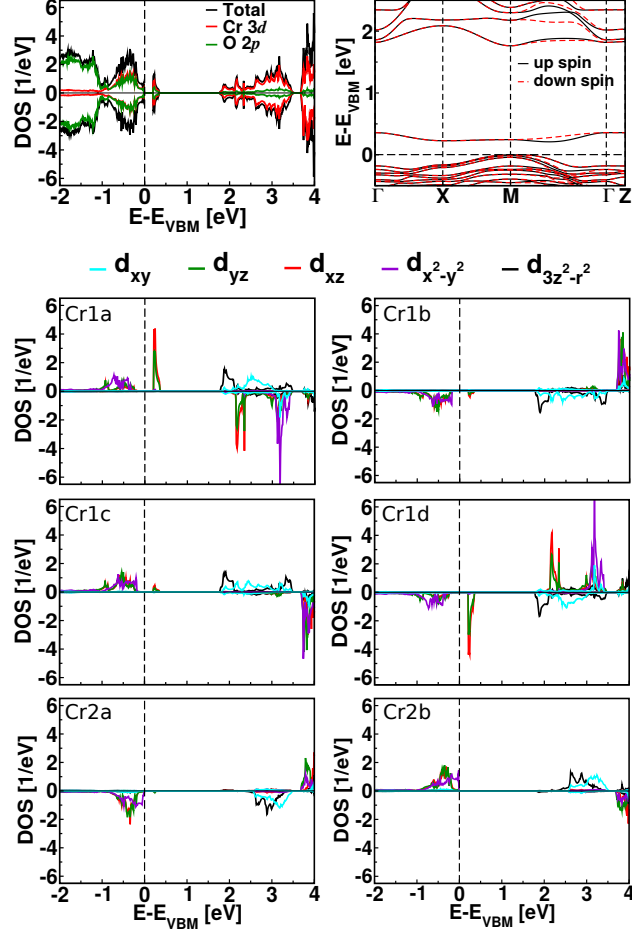


FIG. S3. Total and partial densities of states (sum over all atoms, divided by the number of Cr atoms) as well as band structure of the $m = 4$ superlattice, along with orbitally projected densities of states of the Cr atoms in layers L1 and L2. The labels of the atoms are indicated in Figure 3.

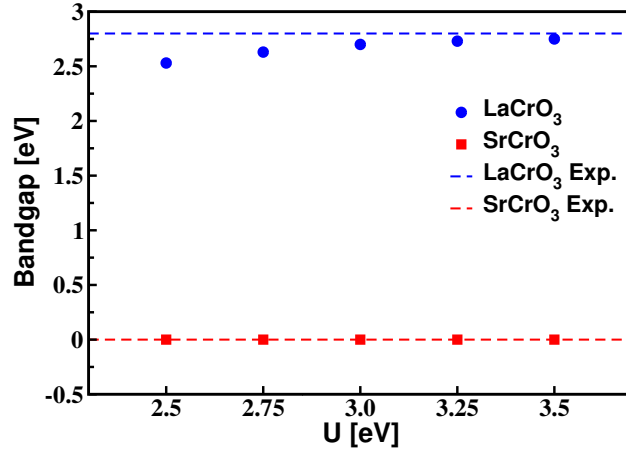


FIG. S4. Effect of the U value on the bandgap.

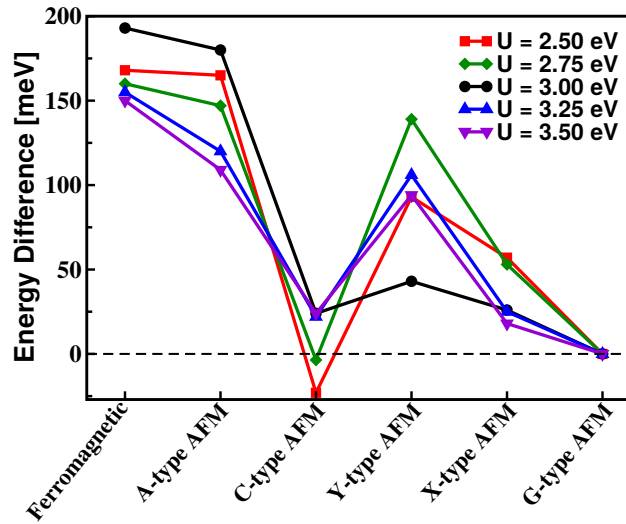


FIG. S5. Effect of the U value on the magnetic ordering.

Relaxed structures in POSCAR format

m=2

1.0

5.4917373657	0.0000000000	0.0000000000
0.0000000000	5.4917373657	0.0000000000
0.0000000000	0.0000000000	11.7875270844

La Sr Cr O

4 2 6 18

Cartesian

5.410919489	0.031924330	1.904257966
5.420596109	5.293623944	5.931861559
2.665147533	2.547337421	5.954241202
2.674712532	2.777381691	1.926569282
5.384508294	5.415808536	9.818696756
2.638629300	2.654916248	9.827172818
5.432664224	2.685512068	11.743138065
5.380170477	2.645664342	7.881781641
2.634311941	5.425166006	11.764133602
2.686769191	5.385365907	7.902777881
5.407230118	2.658409873	3.931114613
2.661331648	5.412495925	3.927299190
0.142030876	2.597515287	1.933222822
5.356403478	2.744155094	9.873835424
5.162086793	2.666046390	5.903891397
2.887800295	5.473557615	5.925154622
2.416193396	5.404555807	1.954493073
2.610618920	5.326731064	9.772064362
3.903950772	1.487919897	0.136786953
3.857976845	1.435314202	7.954038244
1.436174760	3.863223339	7.657950786
1.418706468	3.861618425	0.000288062

1.158320224	1.091474641	7.721764350
1.111818554	1.143517814	11.691882619
4.182340007	4.207920103	0.200327175
4.164217212	4.208901120	7.857894237
1.538844246	3.787135752	4.121127286
3.789508917	1.537197924	3.729246062
4.284713420	4.283755316	3.737475866
1.043595881	1.041923127	4.129024413

m=3

1.0

5.4917373657	0.0000000000	0.0000000000
0.0000000000	5.4917373657	0.0000000000
0.0000000000	0.0000000000	15.7579698563

La Sr Cr O

6 2 8 24

Cartesian

5.485353062	0.124511756	1.896825820
5.474080366	0.132224183	9.884882823
0.047323266	5.307826598	5.898593257
2.717954702	2.561956770	5.904472481
2.782933259	2.878089960	1.918196534
2.771659909	2.870384868	9.906251659
0.049053196	5.401514883	13.771787720
2.716214927	2.655645218	13.789278400
0.021033253	2.745698470	15.729164993
5.488593659	2.734274546	7.887427830
2.741466872	5.490783845	15.681302783
2.759028781	5.477024400	7.887023014
0.006253179	2.731155880	3.916031688
0.023801655	2.744916635	11.879759580
2.768420948	5.480142247	3.915625228

2.744237582	5.491566498	11.831901127
0.361921398	2.678110741	1.941699342
0.345667348	2.704902951	9.884791716
5.118098140	2.800882567	5.903838019
5.229090232	2.775745680	13.717396796
3.138919086	0.055012754	5.899222084
3.027917828	0.029873230	13.843671202
2.419603388	5.450776871	1.918282006
2.403358176	5.423981387	9.861377198
3.972581057	1.462215905	0.265092882
3.915667659	1.569841050	8.183862075
1.584512935	3.897066958	7.591152319
1.549265057	4.024029958	15.592030999
1.169609532	1.151297621	7.603815263
1.249882317	1.232035219	15.531292636
4.238134253	4.242295639	0.276017807
4.334492594	4.314293853	8.178523388
1.595666482	3.897169413	4.199247188
1.515391487	3.977900219	12.029770666
3.922530524	1.568418133	3.624539532
4.018869552	1.496432357	11.527073761
4.341344657	4.315704659	3.619201315
4.284434859	4.208090971	11.537995339
1.180768234	1.151199257	4.211911541
1.215997536	1.278154728	11.969035121

m=4

1.0

5.4917373657	0.0000000000	0.0000000000
0.0000000000	5.4917373657	0.0000000000
0.0000000000	0.0000000000	19.7462329865

La Sr Cr O

8 2 10 30

Cartesian

5.403286082	0.042113737	1.886224999
5.365851619	0.086673916	9.895472985
5.441103852	5.234500066	5.902772406
5.429225263	5.274485108	13.880319074
2.619956750	2.486242506	5.901550125
2.657425910	2.530789589	13.910753092
2.683331539	2.790171248	1.916710068
2.695277886	2.830154980	9.894208922
5.376375050	5.413864832	17.761021220
2.630461195	2.650711327	17.782252531
5.436609569	2.687001434	19.690590685
5.404836004	2.661529030	7.898770488
5.371359980	2.637163176	15.824984320
2.625483114	5.427444244	19.718282369
2.658958647	5.403123398	7.898277927
2.690780330	5.377594365	15.852680713
5.389876884	2.655087770	3.928111562
5.421992184	2.658245879	11.870059092
2.676092241	5.406412440	3.926964313
2.644040607	5.409578078	11.868919787
0.187376427	2.570980524	1.933862747
0.297033307	2.599418074	9.879982920
5.343530778	2.767298851	17.825797964
5.023699215	2.737588302	5.913548717
5.112189451	2.647486115	13.844345072
3.042865820	5.465145156	5.917053137
2.933266857	0.001851699	13.863165954
2.366303911	5.417146019	1.952675832
2.277842644	5.327139903	9.883503229
2.597708577	5.297270107	17.717485203

3.907367475	1.486398453	0.135582438
3.824652049	1.492931693	8.207430137
3.858875047	1.421959831	15.942729296
1.491327107	3.826708355	7.584281909
1.427595852	3.860383070	15.583362369
1.410297118	3.865885539	19.738548568
1.078769372	1.079971094	7.589557665
1.161487908	1.086431093	15.661472975
1.113014547	1.150941237	19.600512677
4.173384502	4.204170503	0.213722127
4.237168294	4.237909703	8.212867137
4.156258109	4.198772454	15.804729892
1.505673296	3.809868706	4.169395723
1.507035002	3.818685749	12.166937299
3.814522400	1.507408816	3.667424213
3.820502447	1.500011744	11.583186283
4.252950002	4.246057023	3.630092285
4.251527740	4.254754589	11.627577955
1.074565270	1.072874186	4.213853600
1.068791442	1.065609765	12.129707472

m=5

1.0

5.4917373657	0.0000000000	0.0000000000
0.0000000000	5.4917373657	0.0000000000
0.0000000000	0.0000000000	23.7141513824

La Sr Cr O

10 2 12 36

Cartesian

5.487392347	0.126328689	1.885874458
5.460936635	0.163501234	9.869260459
5.472840101	0.133899831	17.830737267

0.052032320	5.308223653	5.884622282
0.044794644	5.307896647	13.850395696
2.720485477	2.562037785	5.887816379
2.713246016	2.562343350	13.853592973
2.784168614	2.879785546	1.907473571
2.796089102	2.909371216	9.868954442
2.769612441	2.872183563	17.852332316
0.049109937	5.403738457	21.717634101
2.716150769	2.657869119	21.734730063
0.021868231	2.747665414	23.674958587
0.012241022	2.735381750	7.880488306
5.485249625	2.735659656	15.832549259
2.742556236	0.001185055	23.626959852
2.755860852	5.480609351	7.880822592
2.757778696	5.478936352	15.831867965
0.007498623	2.733080599	3.906345523
0.009427242	2.734734940	11.857395136
0.022706895	2.747047082	19.825398658
2.771760073	5.481539959	3.905664936
2.753047751	5.481243723	11.857728716
2.743396500	0.001788586	19.777397096
0.363257080	2.679322527	1.931298551
0.405367168	2.663478626	9.869610294
0.343866525	2.707426034	17.829940068
5.115555744	2.806905823	5.895622287
5.108404172	2.802242964	13.844847812
5.229118710	2.777636683	21.663119252
3.148613709	0.056384515	5.893365676
3.141464428	0.061025883	13.842591908
3.027881494	0.031769885	21.789246325
2.421399629	5.453304537	1.908268826
2.359919116	5.409348618	9.868605314

2.402010710	5.425181390	17.806908930
3.973675659	1.464074993	0.253947798
3.925283068	1.566536786	8.190633383
3.914681732	1.570360036	16.131951231
1.588457790	3.904041444	7.566157933
1.581219147	3.899340941	15.537868290
1.549869478	4.026343875	23.538421281
1.180349821	1.158201812	7.566041322
1.167850526	1.153602537	15.551149287
1.250924137	1.234222459	23.476871574
4.239068135	4.244241306	0.265166118
4.333399629	4.311742619	8.192749353
4.331783258	4.315377326	16.124162991
1.597425242	3.899483658	4.187063848
1.584937486	3.904063048	12.172172873
1.514327164	3.980096952	19.975494003
3.925226439	1.569522064	3.614048730
3.923624144	1.565869354	11.545464135
4.017944509	1.498353638	19.473038072
4.342331239	4.316243449	3.606261904
4.331744960	4.312402523	11.547580812
4.283316690	4.209927309	19.484256812
1.184054167	1.153482242	4.200344138
1.176824935	1.158162368	12.172056968
1.215403999	1.280476501	19.913944296

m=6

1.0

5.4917373657	0.0000000000	0.0000000000
0.0000000000	5.4917373657	0.0000000000
0.0000000000	0.0000000000	27.7040615082

La Sr Cr O

12 2 14 42

Cartesian

5.398925351	0.053748164	1.881878430
5.359484337	0.100436338	9.884320085
5.361095798	0.096787075	17.848380584
5.434635096	5.247490605	5.898074504
5.440536257	5.241726270	13.863715287
5.424528688	5.285821634	21.833128445
2.615181452	2.499286729	5.897937034
2.613650842	2.495789502	13.862055740
2.652982037	2.542037571	21.864347748
2.678595357	2.801675368	1.913130758
2.694649243	2.846219505	9.882669620
2.688848574	2.840318999	17.848260040
5.370982565	5.425604959	25.714211576
2.625032213	2.662141797	25.736253004
5.431465530	2.698812429	27.644208824
5.402000645	2.673728406	7.896521056
5.397409145	2.670533962	15.850094207
5.366450312	2.648373514	23.778509118
2.620618781	5.439279625	27.671876200
2.651482851	5.417355512	7.896274188
2.656168787	5.414170234	15.849838257
2.685639237	5.388810433	23.806166586
5.385063778	2.667427408	3.924296171
5.399615042	2.670806303	11.873227131
5.416837016	2.669042306	19.823154232
2.670938219	5.418683175	3.923160909
2.653746523	5.417118195	11.873167684
2.639250579	5.420283833	19.822013190
0.181611069	2.581567293	1.929904982
0.303279149	2.598764390	9.884407604

0.291557741	2.612115814	17.832612409
5.338738295	2.780446837	25.779356647
5.019576783	2.752499796	5.910681283
5.003855958	2.740201075	13.861317613
5.107849670	2.656553077	21.797848618
3.037317524	5.475651565	5.913740299
3.049161744	5.489134086	13.861974827
2.927579445	0.014128017	21.816440501
2.362068548	5.431263893	1.948470444
2.257977619	5.347767123	9.885072248
2.273724139	5.335390333	17.835662343
2.592813802	5.307145418	25.671048487
3.902492176	1.498105847	0.130369262
3.821102122	1.505139580	8.199419794
3.821829783	1.500847261	16.167724936
3.853695983	1.433326635	23.897402051
1.485718418	3.840735558	7.583145703
1.484746567	3.838165994	15.536836096
1.422625954	3.871528106	23.536076518
1.405016745	3.878024685	27.693915978
1.075862573	1.095267367	7.578637680
1.075320100	1.091074558	15.546894108
1.156294442	1.097418846	23.615847072
1.108287203	1.162994622	27.552994826
4.168123605	4.215728633	0.210329830
4.230609521	4.249777163	8.209572755
4.231599704	4.247122164	16.163236727
4.151359570	4.210085739	23.756707126
1.500938915	3.821953187	4.163388622
1.484616452	3.840135229	12.186088106
1.501854792	3.829571210	20.120825809
3.809312567	1.519896245	3.665952560

3.822928313	1.501951519	11.559201170
3.815499489	1.510772818	19.536737852
4.247821348	4.258269819	3.625510385
4.230480552	4.247798107	11.560294324
4.246752933	4.265670492	19.582727951
1.069487843	1.085135673	4.209559950
1.077077960	1.094244042	12.187229974
1.063629155	1.076235160	20.080539269