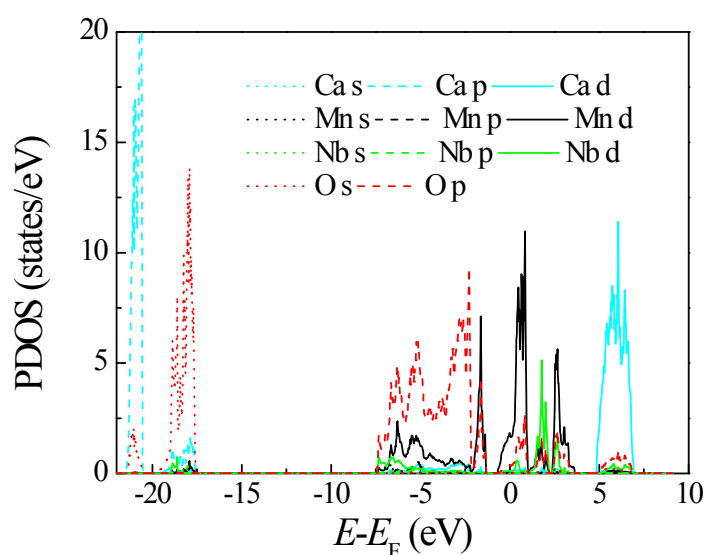


Electron localization in niobium doped CaMnO_3 due to the energy difference of electronic states of Mn and Nb

Yi Li, Jian Liu*, Ji-Chao Li, Yu-Fei Chen, Xin-Miao Zhang, Xue-Jin Wang, Fu-Ning Wang, Wen-Bin Su, Lan-Ling Zhao, Chun-Lei Wang*

School of Physics, Shandong University, 27 Shanda Nanlu, Jinan 250100, P. R. China

1. Bonding features of $\text{CaMn}_{0.75}\text{Nb}_{0.25}\text{O}_3$



The PDOS of *s*, *p* and *d* orbitals are shown in the above figure. The PDOS of Ca *p* orbital overlap that of O *s* orbital in the energy range from -22 eV to -17 eV, but the peaks of their PDOS are at different energy level. The results indicate an ionic bonding feature of Ca-O. In contrast, the PDOS peaks of Mn and O possess the same energy levels at -6.29 eV and 0.85 eV, indicating a covalent interaction between Mn and O.

* Corresponding authors.

Tel.: +86 531 88377098; fax: +86 531 88377032.

E-mail: liujjx@sdu.edu.cn (Jian Liu), wangcl@sdu.edu.cn (Chunlei Wang).

The two energy levels correspond to the bonding state and the anti-bonding state, respectively. Similarly, Nb also shows a covalent interaction with O.

2. POSCAR

CaMn_{0.75}Nb_{0.25}O₃ unit cell

```

1. 000000000000000
   5. 3686401703722275    0. 0088916389550207    0. 0024110198116741
   0. 0125512224523350    7. 5541585848485440    0. 0035096676821194
   0. 0024621118657015    0. 0025427898206253    5. 3023795401382925

```

0 Ca Mn Nb

12 4 3 1

Direct

```

0. 2892148975641831    0. 0395805084377908    0. 7145935465638322
0. 2153413180043177    0. 9615044362368225    0. 2084528746056885
0. 7042145384275100    0. 5393763311420409    0. 3078300573017292
0. 8057975896710540    0. 4600471710001978    0. 7959872981464493
0. 7107851090355340    0. 9604194775105230    0. 2854064436121601
0. 7846586765489694    0. 0384955563929219    0. 7915471235227745
0. 2957854559596185    0. 4606236766980829    0. 6921699450404490
0. 1942024155435505    0. 5399528439544449    0. 2040127147882862
0. 4841616926424343    0. 2442242045097639    0. 0757622645666347
0. 0180268836346545    0. 7461095798855936    0. 5772402790970826
0. 5158383131061928    0. 7557757860703542    0. 9242377270815265
0. 9819731082269487    0. 2538904248532901    0. 4227597265090473
0. 0392720763173462    0. 2347732187524396    0. 9932958815314675
0. 4519560116144186    0. 7638810277219900    0. 4919375323314075
0. 9607279221899728    0. 7652267811418926    0. 0067041161062270
0. 5480439859187258    0. 2361189691650394    0. 5080624675246037
-0. 0000000014376744    -0. 0000000011312493    0. 5000000000242112
0. 4999999995064274    -0. 0000000032043865    -0. 0000000023404752
0. 0000000011278636    0. 5000000044085777    0. 5000000006940558
0. 5000000063979517    0. 5000000064538719    0. 0000000032928422

```

CaMn_{0.75}Nb_{0.25}O₃ supercell

```

1. 000000000000000
   10. 7217435071921461    -0. 0000106614406114    -0. 0030569172842581
   0. 0000205864892176    7. 5677883789633507    0. 0000007388873357
   -0. 0031759431945120    -0. 0000278175848779    10. 6214985662229715
0 Ca Mn Nb

```

Direct

0.1442065890188988	0.0308171405357952	0.3533471366280221
0.1018394426395192	0.9587017187597601	0.1053425933544786
0.3500230358324558	0.5508445077192806	0.1473518947469140
0.3947934678623988	0.4619010275358039	0.4013353126575153
0.3500139343853637	0.9491607350858570	0.1473472388451286
0.3947890505703951	0.0380973963324554	0.4013421779366325
0.1441955246920789	0.4691779364963644	0.3533452242248272
0.1018378883888858	0.5412991046329069	0.1053465180989293
0.2371780426978510	0.2499961361071305	0.0364637692076428
-0.0032893991921314	0.7500028570036144	0.2857390455821516
0.2544531222288462	0.7500043848841627	0.4603968121956974
0.4773779517835923	0.2500119069229180	0.2025597330482722
0.6499918274273120	0.0508196338859590	0.3526812779212377
0.6052190052992084	0.9619257779608366	0.0986683155624473
0.8557845327018979	0.5308279572453338	0.1466482131984647
0.8981518451026617	0.4587281307437935	0.3946705925992437
0.8557930531015480	0.9691633995910884	0.1466502593032763
0.8981556503310080	0.0412847297191213	0.3946704482221149
0.6499899472947576	0.4491725678958786	0.3526765802109148
0.6052241944395388	0.5380690907210721	0.0986682284351466
0.7455588781872710	0.2499979698285595	0.0396076313046346
0.5226078993283724	0.7499872409658536	0.2974389700585636
0.7628146788453088	0.7500013022703912	0.4635335005933923
0.0033007332585720	0.2499963065996514	0.2142794793873467
0.1442045150253712	0.0308269680580955	0.8533453903373490
0.1018359620171010	0.9587102739085472	0.6053357597372327
0.3500186498223191	0.5508264938729139	0.6473418458691430
0.3947903278529605	0.4618990436820021	0.9013301267011605
0.3500116423339282	0.9491723684704017	0.6473370153144182
0.3947915640023724	0.0381014027281103	0.9013323252234618
0.1441981180627105	0.4691757097826476	0.8533419558860259
0.1018361643835828	0.5412955492167673	0.6053389260839106
0.2371698739645814	0.2499956106307647	0.5364569341214016
-0.0032894999682005	0.7500023903329719	0.7857365904143311
0.2544545471049776	0.7500048844904399	0.9603933768536769
0.4773843740573095	0.2500049165544657	0.7025453927479104
0.6499881291455223	0.0508189749585779	0.8526659672863798
0.6052264156255982	0.9619276163719206	0.5986570073040743
0.8557885753073595	0.5308282338059160	0.6466358907611380
0.8981484866359410	0.4587245695991924	0.8946707569892610
0.8557870847365426	0.9691665356594579	0.6466358931763134
0.8981549017261565	0.0412882856124003	0.8946605834064453

0. 6499860100456996	0. 4491765343994805	0. 8526650571215368
0. 6052288773905030	0. 5380776500062839	0. 5986541301672954
0. 7455691229147643	0. 2500006391462132	0. 5396042779364418
0. 5226036132566318	0. 7499948540375536	0. 7974247906186334
0. 7628083183862108	0. 7499982778390749	0. 9635298378352838
0. 0032964172386172	0. 2499959717061338	0. 7142736219446880
0. 0191352840621023	0. 2500014583443261	0. 4977480323989302
0. 2131760226856752	0. 7500001778640387	0. 2465234173342556
0. 4694746371211349	0. 7500030335430693	0. 0058235171959164
0. 2481351816346779	0. 2500013221108541	0. 2513085411669614
0. 5305344321146801	0. 2500013566806593	0. 4941683480612493
0. 7518510764949800	0. 7499993563442711	0. 2486948991688367
0. 9808590554850148	0. 7500017083551833	0. 0022620074415553
0. 7868344205668478	0. 2499982265170434	0. 2534826603397703
0. 0191366166267055	0. 2500009075319956	0. 9977469787847969
0. 2131778144085877	0. 7499974660666128	0. 7465193127226896
0. 4694703834602305	0. 7500025755430343	0. 5058251467781024
0. 2481328530041898	0. 2499994665725361	0. 7512914247379563
0. 5305257352024416	0. 2500002273662332	0. 9941757452966937
0. 7518536359639288	0. 7499984419887326	0. 7486926718758184
0. 9808665222593469	0. 7499995641769315	0. 5022572819696560
0. 7868337716075465	0. 2499929701432749	0. 7534770578376625
0. 0000022969437112	-0. 0000125214008866	0. 2500050281790142
0. 2419921031133287	-0. 0015141468442466	0. 0010802319560805
-0. 0000018468070831	0. 5000118678108330	0. 2500038074939901
0. 2419899906636765	0. 5015146628498385	0. 0010801372916614
0. 2419860193661482	0. 5015134624066152	0. 5010775243353949
0. 7580090882565120	0. 0015159007017174	-0. 0010805470567459
0. 7580052406021552	0. 4984843112904907	-0. 0010807265134673
-0. 0000007000730985	-0. 0000078027165031	0. 7499975399213438
0. 2419866859912216	-0. 0015153214238405	0. 5010789271673780
-0. 0000026388162375	0. 5000068620426168	0. 7499994583892484
0. 7580133585339291	0. 4984859265660612	0. 4989158857486731
0. 7580126658866542	0. 0015149911115946	0. 4989149512135715
0. 5000014584675067	0. 4999857171516988	0. 2499994148499899
0. 4999972642613797	0. 0000149911713059	0. 2500012150970193
0. 5000052476231598	0. 4999983508156217	0. 7499922135454967
0. 5000032359947708	0. 0000017750043668	0. 7499934881099944

CaMn_{0.875}Nb_{0.125}O₃ supercell

1. 00000000000000

10. 6578682268375413	-0. 0000218131546484	0. 0000918007435452
-0. 0000137562515881	7. 5017646819162609	0. 0000117537022184
-0. 0000078380810517	0. 0000139806023962	10. 5323031717361459

O Ca Mn Nb
48 16 14 2

Direct

0.1439721650551564	0.0395889748432828	0.3535334412890344
0.1034864565571564	0.9586143937704088	0.1050594296343285
0.3537090554805735	0.5331359054076928	0.1474637690737746
0.3958500768249568	0.4700906402500452	0.3974930567195394
0.3537102043622931	0.9668663216182631	0.1474650410628086
0.3958477764976758	0.0299043954318348	0.3974981678805095
0.1439716033250938	0.4604086909744931	0.3535323741437193
0.1034928906748969	0.5413885273155975	0.1050572337647653
0.2351738391629373	0.2500097972904372	0.0396981082792364
0.0064228828907146	0.7499990355602543	0.2870330750241266
0.2510722535066374	0.7499979723082720	0.4581778383924999
0.4920747163191289	0.2500024942930975	0.2231311161284404
0.6462913957470999	0.0331329617414191	0.3525364636353801
0.6041499007235851	0.9700958449082672	0.1025033765739256
0.8560293584636053	0.5395929918184071	0.1464716493318430
0.8965069275789095	0.4586129344805546	0.3949425675927321
0.8560294430900566	0.9604093618496224	0.1464720778444009
0.8965111594851001	0.0413846127409520	0.3949422723803792
0.6462894499115107	0.4668652545189102	0.3525365777425243
0.6041479117998714	0.5299094906948418	0.1025091889403908
0.7489276375738171	0.2500056844043447	0.0418273398227142
0.5079261794645094	0.7499972320626075	0.2768696759436671
0.7648266135033850	0.7499967145387544	0.4603044822391180
0.9935759056910238	0.2500005847854377	0.2129678046926484
0.1442540433296045	0.0299525514747058	0.8556092099204876
0.1047565663939145	0.9616828965056661	0.6051267269082015
0.3517352521921777	0.5518555827795606	0.6430682114525711
0.3900556957446049	0.4525640795302284	0.8978594119335382
0.3517359619239154	0.9481469898565590	0.6430628038441847
0.3900571233949408	0.0474322117622991	0.8978559066819934
0.1442548208816001	0.4700531912998583	0.8556063803552927
0.1047500102406281	0.5383184501860734	0.6051255647344259
0.2449339205654737	0.2500010942574821	0.5342380263677415
0.9970060201903257	0.7499945063733775	0.7850743568097769
0.2605454121174726	0.7499930074342632	0.9659229368893968
0.4832207056237110	0.2500013877188659	0.6948903978379350
0.6482644802637477	0.0518589147641366	0.8569323250056821
0.6099431329214839	0.9525669990071780	0.6021423017048463
0.8557459063791333	0.5299455731826398	0.6443932695806117
0.8952516167289354	0.4616814669237887	0.8948721066472625
0.8557442218155489	0.9700480946302149	0.6443898466262876

0. 8952459417093500	0. 0383169401859550	0. 8948703431074614
0. 6482613567140718	0. 4481429303743771	0. 8569303670664788
0. 6099441682445089	0. 5474334804656303	0. 6021411160008624
0. 7394546264457967	0. 2500000269322565	0. 5340750573875090
0. 5167789244836055	0. 7499993620486602	0. 8051069268140284
0. 7550655316701406	0. 7499949852588942	0. 9657581206560497
0. 0029934087231930	0. 2500054354160933	0. 7149250805081089
0. 0227331518579584	0. 2500036096736708	0. 4952249276006487
0. 2255763119461051	0. 7499966667447837	0. 2423336460602955
0. 4752930241984356	0. 7499975263962348	0. 0223748289099292
0. 2706338864283699	0. 2500027735013218	0. 2560842292439767
0. 5247085537035056	0. 2499983584187908	0. 4776256805223107
0. 7293681514440556	0. 7499982606468043	0. 2439217378018726
0. 9772714335154116	0. 7499969574500098	0. 0047738575675800
0. 7744259497490142	0. 2500027275934555	0. 2576708310495460
0. 0175678173304605	0. 2499989409728817	0. 9977135240508971
0. 2168709909469285	0. 7499980899072920	0. 7495317902218538
0. 4762236491340082	0. 7499988781183802	0. 4897051107460016
0. 2499299356105996	0. 2500038689833713	0. 7508170982999199
0. 5237703266528405	0. 2500027213150798	0. 0102970090642271
0. 7500704139401275	0. 7499981532678622	0. 7491776651317881
0. 9824310731493674	0. 7500036368656072	0. 5022859542110948
0. 7831292400863038	0. 2500008639487978	0. 7504632276574692
-0. 0000001117873048	0. 9999973748284637	0. 2499991367230548
0. 2461305327893708	0. 0017836103170287	0. 0043835154954067
-0. 0000005757697244	0. 4999994445219641	0. 2500004375386143
0. 2461293389915799	0. 4982150484140562	0. 0043825954402723
0. 7538708489670871	0. 5017853984964269	0. 4956174626027575
0. 7536771782098802	0. 0031165497851356	0. 0031313750651033
0. 7536779788705034	0. 4968851483601037	0. 0031302406697350
0. 0000012983949829	0. 0000012793989278	0. 7499985812077644
0. 2463236379539905	0. 9968838598281957	0. 4968693731277465
-0. 0000000878610825	0. 5000004481890001	0. 7500000605398305
0. 4999997804721356	-0. 0000014676297639	0. 2500015576222271
0. 7538709863268322	0. 9982165039329113	0. 4956149061343739
0. 5000009277735007	0. 4999991651841598	0. 2500005041682016
0. 2463220385613464	0. 5031155839664920	0. 4968700448699530
0. 4999976307124326	0. 5000000643193069	0. 7499998587859869
0. 5000000353133839	-0. 0000010216933296	0. 7499963088963202