# Supporting Information

# Developing and optimizing novel $Cr^{3+}$ activated inorganic NIR phosphors by combining triple-objective optimization and crystal field engineering

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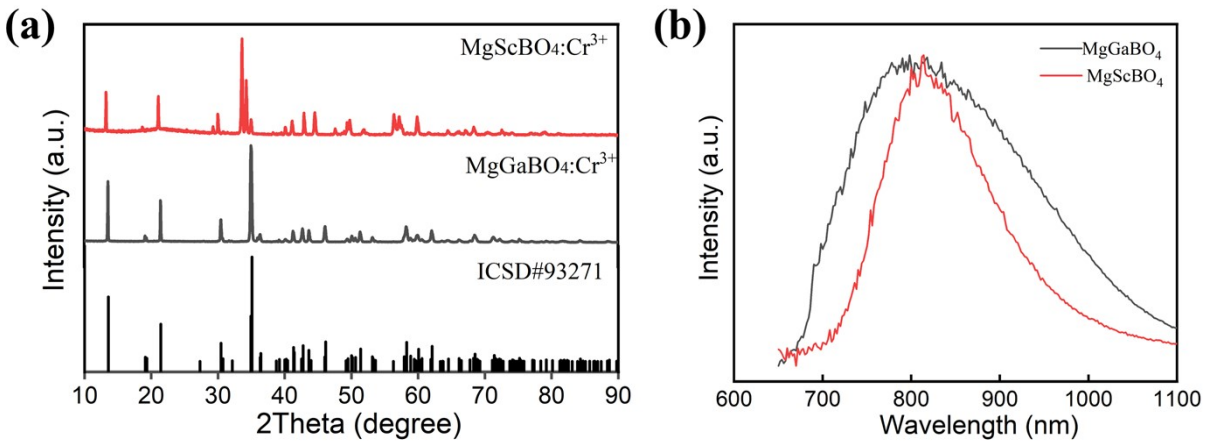


**Figure S1.** XRD patterns and emission spectra of $MgMBO_4$ (M = Ga, Sc).

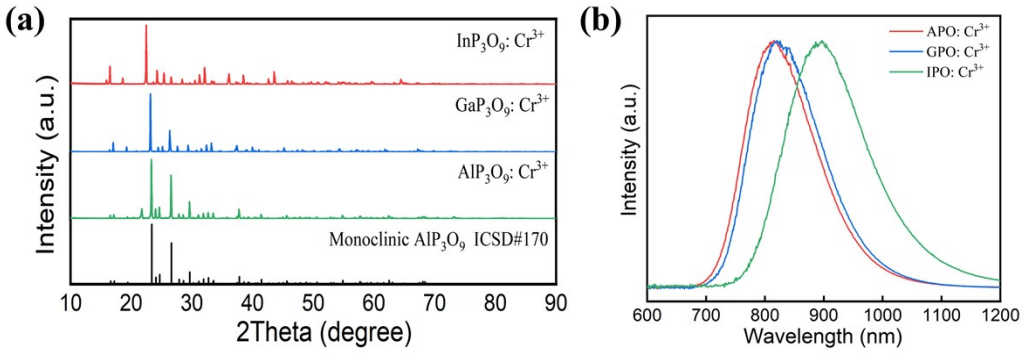


**Figure S2**. XRD patterns and emission spectra of $MP_3O_9$: $Cr^{3+}$ (M = Al, Ga, In).

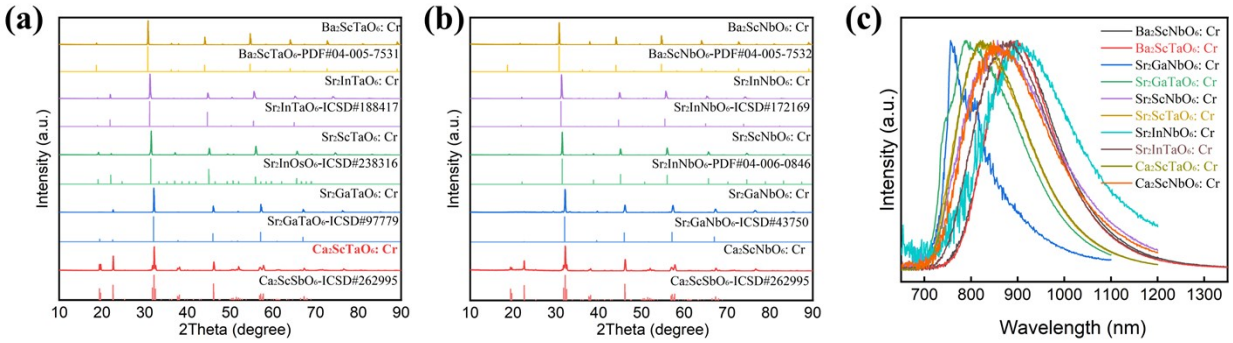


**Figure S3**. XRD patterns and emission spectra of $A_2MM'O_6$: $Cr^{3+}$ (A = Ca, Sr, Ba; M = Sc, In, Ga, Al; M' = Nb, Ta).

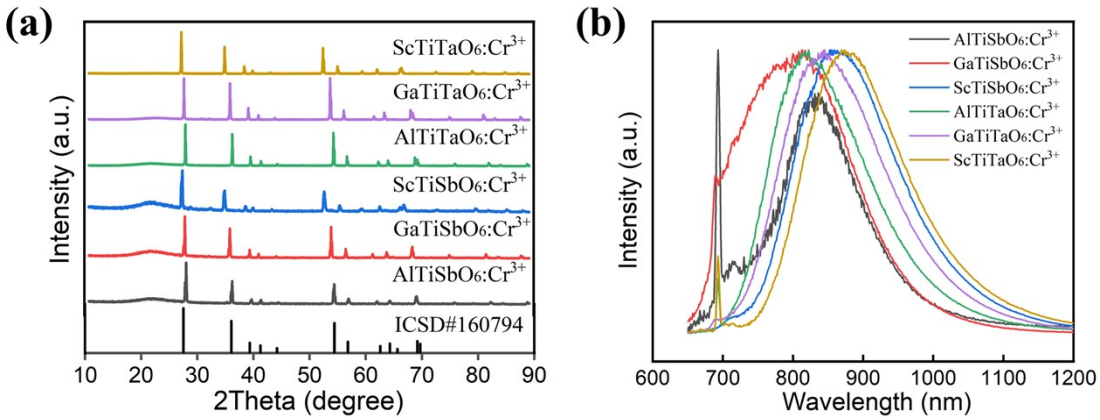


**Figure S4.** XRD patterns and emission spectra of MTiAO6 (M = Al, Ga, Sc, A= Sb, Ta).

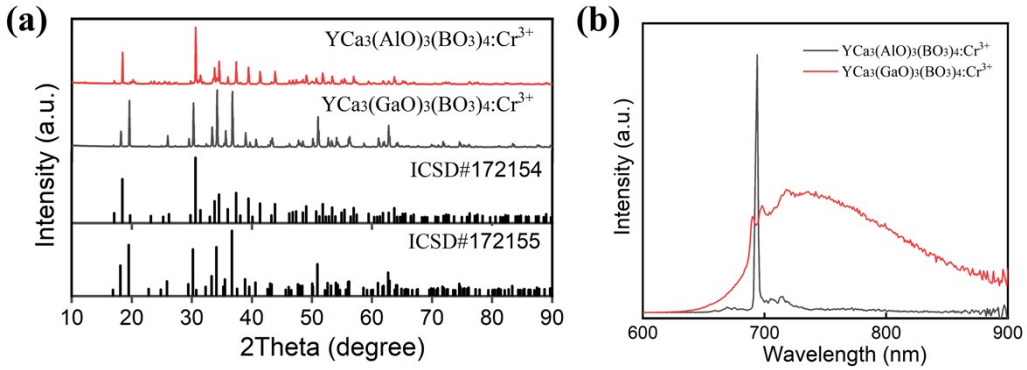


**Figure S5.** XRD patterns and emission spectra of $Ca_3Y(MO)_3(BO_3)_4$ (M = Al, Ga).

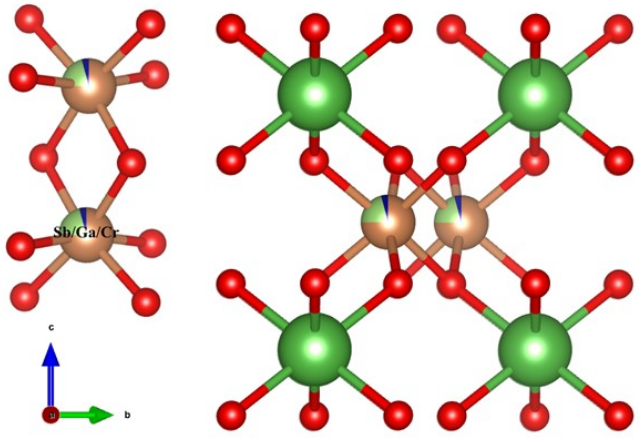


**Figure S6. Crystal structure of LGS:Cr.**

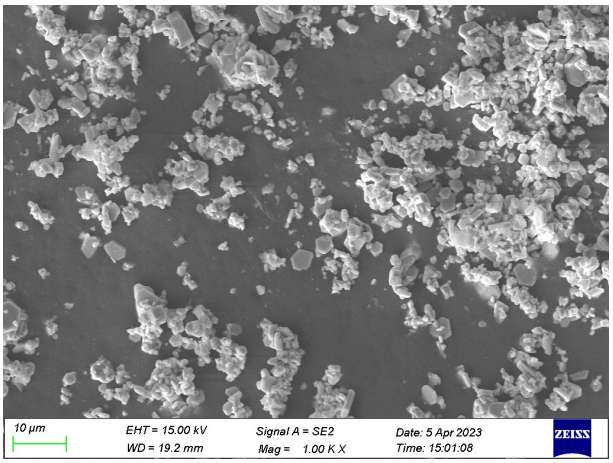


**Figure S7.** SEM image of LGS:0.04$Cr^{3+}$.

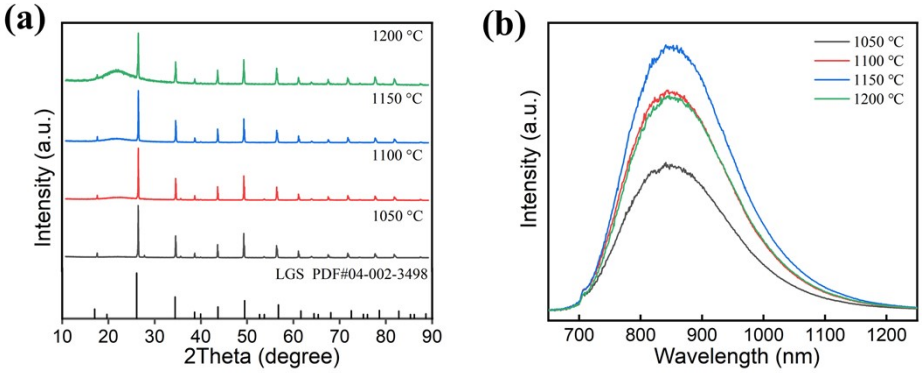


**Figure S8.** XRD patterns and emission spectra of LGS:0.04$Cr^{3+}$ at different synthesis temperature.

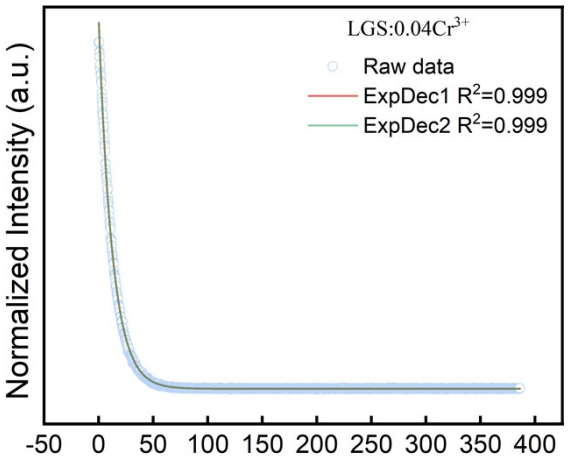


**Figure S9.** Fitting of decay curves using single and double exponential functions.

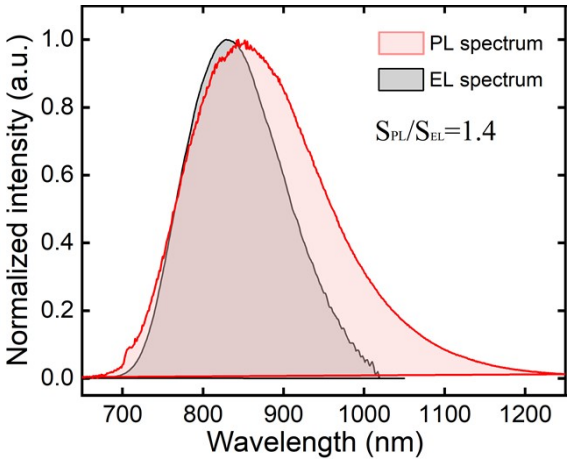


**Figure S10.** Comparison of EL and PL spectrum of LGS: $Cr^{3+}$ phosphors

## Table S1 IQE dataset.

| TIE | Va | Hf | Mb | IQE | Pretty formula | DOI |
|---|---|---|---|---|---|---|
| 46.0065 | 1.6139 | 0.12705 | 13.175 | 91 | GdAl3B4O12 | 10.1039/d0tc04803h |
| 55.58571 | 1.929857 | 0.052357 | 7.628571 | 35 | Mg3Ga2GeO8 | 10.1021/acsaelm.9b00219 |
| 62.1723 | 2.4568 | 0.021 | 7.52 | 75 | Na3AlF6 | 10.1021/acsaelm.9b00527 |
| 52.9454 | 2.1377 | 0.1235 | 5.28 | 45.9 | CaMgSi2O6 | 10.1016/j.materresbull.2021.111725 |
| 48.60287 | 2.201256 | 0.025144 | 2.746667 | 58.3 | Ca2LaZr2Ga2.8Al0.2O12 | 10.1021/acsaelm.1c01029 |
| 47.34836 | 2.289273 | 0.014818 | 6.836364 | 78.9 | KAlP2O7 | 10.1021/acsami.2c00200 |
| 45.37654 | 1.82576 | 0.024208 | 0 | 87.9 | Ga1.96In0.04O3 | 10.1021/acsami.1c05949 |
| 54.5668 | 1.9082 | 0.1253 | 5.66 | 64 | LiScSi2O6 | 10.1021/acsami.1c23940 |
| 49.4677 | 2.0846 | 0.1249 | 5.66 | 22 | NaScSi2O6 | 10.1021/acsami.1c23940 |
| 57.50614 | 1.981429 | 0.076571 | 8.085714 | 26 | LiScGeO4 | 10.1021/acsami.1c10490 |
| 46.8812 | 2.1211 | 0.09 | 14.9 | 21 | CaScAlSiO6 | 10.1021/acs.chemmater.1c04131 |
| 47.55445 | 2.315364 | 0.01 | 0 | 74.4 | KGaP2O7 | 10.1021/acs.chemmater.1c03671 |
| 46.91886 | 2.161214 | 0.134643 | 6.414286 | 7 | BaZrSi3O9 | 10.1039/d1qi01082d |
| 48.11857 | 2.103571 | 0.1245 | 4.957143 | 16 | BaSnSi3O9 | 10.1039/d1qi01082d |
| 46.94114 | 2.155 | 0.138 | 7.785714 | 13 | BaHfSi3O9 | 10.1039/d1qi01082d |
| 47.34485 | 1.767769 | 0.011538 | 5.784615 | 76 | AlP3O9 | 10.1039/d2qi00046f |
| 46.43494 | 1.889563 | 0.026 | 1.1125 | 82.6 | LaMgGa11O19 | 10.1039/d0qi00063a |
| 45.398 | 1.8204 | 0.0244 | 0 | 92.4 | Ga2O3 | 10.1039/d0tc02705g |
| 45.33131 | 1.767389 | 0.133461 | 7.6693 | 41 | Y0.57La0.72Sc2.71(BO3)4 | 10.1039/d1tc01508g |
| 54.8954 | 1.9199 | 0.1121 | 0 | 75 | LiInSi2O6 | 10.1016/j.cej.2019.123108 |
| 59.381 | 1.979429 | 0.074143 | 10.17143 | 48.19 | Mg2GeO4 | 10.1039/d1tc00521a |
| 46.3112 | 1.7228 | 0.112 | 0 | 46.3 | InBO3 | 10.1016/j.ceramint.2021.01.218 |
| 47.271 | 2.255 | 0.0452 | 12.54 | 58 | La2MgZrO6 | 10.1021/acs.chemmater.9b01587 |
| 45.654 | 1.6994 | 0.1384 | 11.32 | 65 | ScBO3 | 10.1039/c8ra01084f |
| 55.041 | 1.9723 | 0.0739 | 0 | 81.2 | LiInGe2O6 | 10.1111/jace.17856 |
| 46.88231 | 2.424769 | 0.024385 | 13.43077 | 48 | K2Ga2Sn6O16 | 10.1111/jace.17157 |
| 54.7124 | 1.9606 | 0.0871 | 5.66 | 72.6 | LiSc1Ge2O6 | 10.1039/d1tc03057d |
| 48.9918 | 2.0549 | 0.0858 | 7.32 | 79 | Y3Mg2AlSi2O12 | |
| 43.26765 | 2.08135 | 0.04435 | 5.66 | 83 | Y3Sc2Ga3O12 | |
| 44.88845 | 2.0965 | 0.0427 | 9.11 | 59 | CaY2ZrAlGa3O12 | |

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|---|---|---|---|---|---|---|
| 46.1448 | 2.0046 | 0.0663 | 13.06 | 80 | Y3MgAlAl2SiO12 | |
| 46.8057 | 1.9635 | 0.05105 | 9.3 | 94 | Y2MgGa2Al2GeO12 | |
| 43.29735 | 2.08015 | 0.0421 | 11.345 | 72 | Gd3Sc2Ga3O12 | |
| 46.8255 | 1.9627 | 0.04955 | 13.09 | 97 | Gd2MgAl2Ga2GeO12 | |
| 43.5542 | 1.9818 | 0.03925 | 16.965 | 95 | Gd3Al3Ga2O12 | |
| 43.98005 | 1.97085 | 0.05005 | 7.14 | 95 | Lu3Ga5O12 | |
| 46.487 | 1.9781 | 0.0775 | 12.68 | 59 | Lu3MgAlGa2SiO12 | |
| 44.4523 | 2.1474 | 0.0725 | 18.54 | 58 | Lu2SrSc2Al2SiO12 | |
| 46.4428 | 2.2017 | 0.0631 | 11.42 | 2 | LuCa2ScZrGa2GeO12 | |
| 43.4133 | 1.8991 | 0.0633 | 25.94 | 95 | Lu3Al5O12 | |
| 48.3705 | 2.32615 | 0.0808 | 8.24 | 2 | Ca3Sc2Ge3O12 | |
| 45.8089 | 2.1522 | 0.05375 | 23.875 | 26 | Ca2Gd1 Zr2Al3O12 | |
| 46.51455 | 2.14535 | 0.063 | 16.11 | 50 | Ca2LuGaZrAl2GeO12 | |
| 46.07195 | 2.2168 | 0.0439 | 10.7 | 13.6 | Ca2LaZr2Ga3O12 | |
| 45.8687 | 2.1255 | 0.0647 | 26.28 | 44 | Ca2LuHf2Al3O12 | |
| 46.4064 | 2.1886 | 0.07265 | 11.42 | 7 | LuCa2ScZrGa2SiO12 | |
| 46.422 | 2.18425 | 0.075 | 12.38 | 20 | LuCa2ScHfGa2SiO12 | |
| 46.4584 | 2.19735 | 0.06545 | 12.38 | 30 | LuCa2ScHfGa2GeO12 | |
| 43.05085 | 2.05225 | 0.0489 | 15.075 | 82 | Y2GdSc2Al2GaO12 | |
| 45.9597 | 2.0466 | 0.06905 | 12.13 | 60 | Y3ScMgAl2SiO12 | |
| 46.2161 | 2.0741 | 0.0615 | 10.295 | 50 | Gd3ScMgGa2SiO12 | |
| 46.3008 | 2.22815 | 0.0645 | 9.04 | 6 | Ca2LaZrScSiGa2O12 | |
| 49.17795 | 2.09545 | 0.06405 | 3.56 | 45 | Y3Mg2GaGe2O12 | |
| 44.8368 | 1.92425 | 0.07305 | 23.07 | 92 | Lu3Al4Mg0.5Si0.5O12 | |
| 47.8036 | 2.26415 | 0.06825 | 11.56 | 8 | Ca3Zr2SiGa2O12 | |
| 48.5556 | 2.28415 | 0.07805 | 9.17 | 1.5 | Ca3AlScGe3O12 | |
| 47.84 | 2.27725 | 0.0587 | 11.56 | 2 | Ca3Zr2Ga2GeO12 | |
| 46.2218 | 1.9678 | 0.0773 | 17.82 | 80 | YLu2Al3MgSiO12 | |
| 47.1531 | 2.1749 | 0.0605 | 5.48 | 34 | Ca2YGa2AlGe2O12 | |
| 46.4376 | 2.0452 | 0.0492 | 11.225 | 75.4 | Gd3MgAlGa2GeO12 | |
| 49.20765 | 2.09425 | 0.0618 | 9.245 | 36.3 | Gd3Mg2GaGe2O12 | |
| 49.0646 | 2.0811 | 0.0667 | 7.32 | 36.5 | Y3Mg2AlGe2O12 | |

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|---|---|---|---|---|---|---|
| 46.3383 | 2.0332 | 0.0707 | 11.75 | 72.5 | Lu3ScMgGa2GeO12 | |
| 46.48485 | 2.04765 | 0.05835 | 1.78 | 80.2 | Y3Ga3MgSiO12 | |

**Table S2 WL dataset.**

| TIE | Va | WL | Pretty formula | DOI |
|---|---|---|---|---|
| 46.0065 | 1.6139 | 740 | GdAl3B4O12 | 10.1039/d0tc04803h |
| 55.58571 | 1.929857 | 918 | Mg3Ga2GeO8 | 10.1021/acsaelm.9b00219 |
| 62.1723 | 2.4568 | 720 | Na3AlF6 | 10.1021/acsaelm.9b00527 |
| 49.00116 | 2.5116 | 870 | Sr8MgLa(PO4)7 | 10.1016/j.optmat.2018.09.001 |
| 52.9454 | 2.1377 | 822 | CaMgSi2O6 | 10.1016/j.materresbull.2021.111725 |
| 48.60287 | 2.201256 | 820 | Ca2LaZr2Ga2.8Al0.2O12 | 10.1021/acsaelm.1c01029 |
| 47.34836 | 2.289273 | 780 | KAlP2O7 | 10.1021/acsami.2c00200 |
| 45.37654 | 1.82576 | 810 | Ga1.96In0.04O3 | 10.1021/acsami.1c05949 |
| 54.5668 | 1.9082 | 845 | LiScSi2O6 | 10.1021/acsami.1c23940 |
| 49.4677 | 2.0846 | 845 | NaScSi2O6 | 10.1021/acsami.1c23940 |
| 47.55445 | 2.315364 | 815 | KGaP2O7 | 10.1021/acs.chemmater.1c03671 |
| 73.77667 | 1.946417 | 750 | Li3Mg2NbO6 | 10.1039/d1ce00746g |
| 45.50118 | 1.9507 | 764 | SrGa11.2Sc0.8O19 | 10.1039/d1dt03461h |
| 46.91886 | 2.161214 | 811 | BaZrSi3O9 | 10.1039/d1qi01082d |
| 48.11857 | 2.103571 | 806 | BaSnSi3O9 | 10.1039/d1qi01082d |
| 46.94114 | 2.155 | 822 | BaHfSi3O9 | 10.1039/d1qi01082d |
| 47.34485 | 1.767769 | 780 | AlP3O9 | 10.1039/d2qi00046f |
| 47.07486 | 2.217357 | 830 | BaZrGe3O9 | 10.1039/d0qi01524e |
| 46.43494 | 1.889563 | 770 | LaMgGa11O19 | 10.1039/d0qi00063a |
| 45.398 | 1.8204 | 714 | Ga2O3 | 10.1039/d0tc02705g |
| 50.589 | 1.815778 | 834 | MgTa2O6 | 10.1039/d0tc01951h |
| 54.8954 | 1.9199 | 840 | LiInSi2O6 | 10.1016/j.cej.2019.123108 |
| 59.381 | 1.979429 | 940 | Mg2GeO4 | 10.1039/d1tc00521a |

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|---|---|---|---|---|
| 46.3112 | 1.7228 | 820 | InBO3 | 10.1016/j.ceramint.2021.01.218 |
| 47.271 | 2.255 | 825 | La2MgZrO6 | 10.1021/acs.chemmater.9b01587 |
| 45.654 | 1.6994 | 800 | ScBO3 | 10.1039/c8ra01084f |
| 48.8072 | 2.321 | 760 | CaTiO3 | 10.1016/j.jallcom.2016.01.135 |
| 53.7399 | 2.3592 | 800 | Ca2MgWO6 | 10.1016/j.jallcom.2017.10.036 |
| 55.041 | 1.9723 | 880 | LiInGe2O6 | 10.1016/j.jallcom.2017.10.036 |
| 54.7124 | 1.9606 | 886 | LiSc1Ge2O6 | 10.1039/d1tc03057d |
| 46.04315 | 1.841538 | 850 | Ga4GeO8 | 10.1002/adom.202102229 |
| 45.56233 | 1.782 | 840 | GaTaO4 | 10.1002/adom.202101800 |
| 43.96555 | 2.156 | 770 | Gd2GaSbO7 | 10.1039/d1dt02259h |
| 49.5935 | 2.4242 | 840 | Ca4ZrGe3O12 | 10.1039/d1qm01540k |
| 48.31062 | 2.557533 | 860 | Sr9Sc(PO4)7 | 10.1021/acs.inorgchem.1c03377 |
| 74.11004 | 1.942885 | 814 | LiGe2(PO4)3 | 10.1016/j.jallcom.2022.163945 |
| 45.42019 | 2.6575 | 761 | Sr3Sc4O9 | 10.1016/j.jallcom.2022.16458 |
| 47.06008 | 1.832385 | 900 | Sc(PO3)3 | 10.1111/jace.18319 |
| 47.07486 | 2.217357 | 820 | BaZrGe3O9 | 10.1016/j.jlumin.2021.118084 |
| 45.8375 | 2.1342 | 780 | Ca2Lu1 Zr2Al3O12 | 10.1002/adom.201901684 |
| 43.38315 | 2.02615 | 707 | Lu3Sc2Ga3O12 | 10.1016/j.jlumin.2018.05.076 |
| 43.26765 | 2.08135 | 729 | Y3Sc2Ga3O12 | 10.1016/j.jlumin.2018.05.076 |
| 43.29735 | 2.08015 | 748 | Gd3Sc2Ga3O12 | 10.1016/j.jlumin.2018.05.076 |
| 43.06635 | 2.1448 | 818 | La3Sc2Ga3O12 | 10.1016/j.jlumin.2018.05.076 |
| 45.0757 | 2.03715 | 744 | Y2Ca1Al4Si1O12 | 10.1039/C9TC05775G |
| 46.60035 | 2.1029 | 760 | Y1Ca2Al3Si2O12 | 10.1039/C9TC05775G |
| 43.2978 | 1.9543 | 703 | Y3Al5O12 | 10.1039/C9TC05775G |
| 45.8687 | 2.1255 | 782 | Ca2LuHf2Al3O12 | 10.1002/adom.201900185 |
| 52.3458 | 2.0616 | 776 | Mg3Y2Ge3O12 | 10.1016/j.ijleo.2021.166305 |
| 48.2613 | 2.28685 | 770 | Ca3Sc2Si3O12 | 10.1016/j.ceramint.2019.04.133 |
| 45.7631 | 2.16505 | 780 | Ca2LaHf2Al3O12 | 10.1039/d0dt03840g |
| 45.8302 | 2.1439 | 775 | Ca2YHf2Al3O12 | 10.1039/d0tc05657j |
| 47.0065 | 2.1985 | 804 | Ca2LuScGa2Ge2O12 | 10.1021/acs.inorgchem.0c01890 |

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|---|---|---|---|---|
| 43.76885 | 2.04995 | 787 | La2LuGa5O12 | 10.1039/c9nj03167g |
| 43.6555 | 2.0356 | 751 | La2LuAl1Ga4O12 | 10.1039/c9nj03167g |
| 43.54215 | 2.02125 | 735 | La2LuAl2Ga3O12 | 10.1039/c9nj03167g |
| 43.4288 | 2.0069 | 735 | La2LuAl3Ga2O12 | 10.1039/c9nj03167g |
| 43.3275 | 1.9531 | 710 | Gd3Al5O12 | 10.1016/j.snb.2018.04.157 |
| 43.44085 | 1.96745 | 719 | Gd3Al4GaO12 | 10.1016/j.snb.2018.04.157 |
| 43.66755 | 1.99615 | 735 | Gd3Al2Ga3O12 | 10.1016/j.snb.2018.04.157 |
| 43.7809 | 2.0105 | 754 | Gd3AlGa4O12 | 10.1016/j.snb.2018.04.157 |
| 43.89425 | 2.02485 | 756 | Gd3Ga5O12 | 10.1016/j.snb.2018.04.157 |
| 43.79806 | 1.9997 | 728 | Gd2.4Lu0.6Ga4AlO12 | 10.1016/j.cej.2021.132003 |
| 47.9451 | 2.40795 | 800 | Ca3Y2Ge3O12 | 10.1016/j.jallcom.2021.158699 |
| 50.8467 | 2.10095 | 750 | CaLu2Mg2Si3O12 | 10.1002/adom.202100388 |
| 43.3899 | 2.05915 | 753 | Gd3ScAlGa3O12 | 10.1002/adom.202000296 |
| 48.9918 | 2.0549 | 768 | Y3Mg2AlSi2O12 | |
| 43.26765 | 2.08135 | 748 | Y3Sc2Ga3O12 | |
| 44.88845 | 2.0965 | 768 | CaY2ZrAlGa3O12 | |
| 46.1448 | 2.0046 | 769 | Y3MgAlAl2SiO12 | |
| 46.8057 | 1.9635 | 750 | Y2MgGa2Al2GeO12 | |
| 43.29735 | 2.08015 | 763 | Gd3Sc2Ga3O12 | |
| 46.8255 | 1.9627 | 738 | Gd2MgAl2Ga2GeO12 | |
| 43.5542 | 1.9818 | 726 | Gd3Al3Ga2O12 | |
| 43.98005 | 1.97085 | 705 | Lu3Ga5O12 | |
| 46.487 | 1.9781 | 769 | Lu3MgAlGa2SiO12 | |
| 44.4523 | 2.1474 | 704 | Lu2SrSc2Al2SiO12 | |
| 46.4428 | 2.2017 | 816 | LuCa2ScZrGa2GeO12 | |
| 43.4133 | 1.8991 | 704 | Lu3Al5O12 | |
| 48.3705 | 2.32615 | 792 | Ca3Sc2Ge3O12 | |
| 45.8089 | 2.1522 | 806 | Ca2Gd1 Zr2Al3O12 | |
| 46.51455 | 2.14535 | 787 | Ca2LuGaZrAl2GeO12 | |
| 46.07195 | 2.2168 | 776 | Ca2LaZr2Ga3O12 | |

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|---|---|---|---|---|
| 45.8687 | 2.1255 | 789 | Ca2LuHf2Al3O12 | |
| 46.4064 | 2.1886 | 825 | LuCa2ScZrGa2SiO12 | |
| 46.422 | 2.18425 | 820 | LuCa2ScHfGa2SiO12 | |
| 46.4584 | 2.19735 | 820 | LuCa2ScHfGa2GeO12 | |
| 43.05085 | 2.05225 | 745 | Y2GdSc2Al2GaO12 | |
| 45.9597 | 2.0466 | 781 | Y3ScMgAl2SiO12 | |
| 46.2161 | 2.0741 | 818 | Gd3ScMgGa2SiO12 | |
| 46.3008 | 2.22815 | 818 | Ca2LaZrScSiGa2O12 | |
| 49.17795 | 2.09545 | 784 | Y3Mg2GaGe2O12 | |
| 44.8368 | 1.92425 | 706 | Lu3Al4Mg0.5Si0.5O12 | |
| 47.8036 | 2.26415 | 832 | Ca3Zr2SiGa2O12 | |
| 48.5556 | 2.28415 | 790 | Ca3AlScGe3O12 | |
| 47.84 | 2.27725 | 830 | Ca3Zr2Ga2GeO12 | |
| 46.2218 | 1.9678 | 734 | YLu2Al3MgSiO12 | |
| 47.1531 | 2.1749 | 790 | Ca2YGa2AlGe2O12 | |
| 46.4376 | 2.0452 | 782 | Gd3MgAlGa2GeO12 | |
| 49.20765 | 2.09425 | 805 | Gd3Mg2GaGe2O12 | |
| 49.0646 | 2.0811 | 771 | Y3Mg2AlGe2O12 | |
| 46.3383 | 2.0332 | 770 | Lu3ScMgGa2GeO12 | |
| 46.48485 | 2.04765 | 774 | Y3Ga3MgSiO12 | |

**Table S3 TS dataset.**

| IR | TIE | Va | TS | Pretty formula | DOI |
|---|---|---|---|---|---|
| 0.352143 | 55.58571 | 1.929857 | 55 | Mg3Ga2GeO8 | 10.1021/acsaelm.9b00219 |
| 0.8395 | 62.1723 | 2.4568 | 70 | Na3AlF6 | 10.1021/acsaelm.9b00527 |
| 0.312 | 52.9454 | 2.1377 | 72 | CaMgSi2O6 | 10.1016/j.materresbull.2021.111725 |
| 0.35864 | 45.6876 | 2.09064 | 70 | La3GaGe5O16 | 10.1039/c4ra09793a |
| 0.3375 | 48.60287 | 2.201256 | 36 | Ca2LaZr2Ga2.8Al0.2O12 | 10.1021/acsaelm.1c01029 |
| 0.317727 | 47.34836 | 2.289273 | 77 | KAlP2O7 | 10.1021/acsami.2c00200 |

| | | | | | |
|---|---|---|---|---|---|
| 0.30944 | 45.37654 | 1.82576 | 60 | Ga1.96In0.04O3 | 10.1021/acsami.1c05949 |
| 0.2905 | 54.5668 | 1.9082 | 75 | LiScSi2O6 | 10.1021/acsami.1c23940 |
| 0.3165 | 49.4677 | 2.0846 | 69 | NaScSi2O6 | 10.1021/acsami.1c23940 |
| 0.376429 | 57.50614 | 1.981429 | 10 | LiScGeO4 | 10.1021/acsami.1c10490 |
| 0.328 | 46.8812 | 2.1211 | 30 | CaScAlSiO6 | 10.1021/acs.chemmater.1c04131 |
| 0.325455 | 47.55445 | 2.315364 | 56 | KGaP2O7 | 10.1021/acs.chemmater.1c03671 |
| 0.42 | 73.77667 | 1.946417 | 20 | Li3Mg2NbO6 | 10.1039/d1ce00746g |
| 0.331875 | 45.50118 | 1.9507 | 80 | SrGa11.2Sc0.8O19 | 10.1039/d1dt03461h |
| 0.297857 | 46.91886 | 2.161214 | 59 | BaZrSi3O9 | 10.1039/d1qi01082d |
| 0.299286 | 48.11857 | 2.103571 | 38 | BaSnSi3O9 | 10.1039/d1qi01082d |
| 0.297143 | 46.94114 | 2.155 | 43 | BaHfSi3O9 | 10.1039/d1qi01082d |
| 0.368571 | 47.07486 | 2.217357 | 53 | BaZrGe3O9 | 10.1039/d0qi01524e |
| 0.32725 | 46.43494 | 1.889563 | 85 | LaMgGa11O19 | 10.1039/d0qi00063a |
| 0.296 | 54.8954 | 1.9199 | 77 | LiInSi2O6 | 10.1016/j.cej.2019.123108 |
| 0.367143 | 59.381 | 1.979429 | 8 | Mg2GeO4 | 10.1039/d1tc00521a |
| 0.274 | 46.3112 | 1.7228 | 55 | InBO3 | 10.1016/j.ceramint.2021.01.218 |
| 0.263 | 45.654 | 1.6994 | 49 | ScBO3 | 10.1039/c8ra01084f |
| 0.362 | 55.041 | 1.9723 | 22 | LiInGe2O6 | 10.1016/j.jallcom.2017.10.036 |
| 0.308462 | 46.04315 | 1.841538 | 56 | Ga4GeO8 | 10.1002/adom.202102229 |
| 0.29 | 45.56233 | 1.782 | 60 | GaTaO4 | 10.1002/adom.202101800 |
| 0.359636 | 43.96555 | 2.156 | 50 | Gd2GaSbO7 | 10.1039/d1dt02259h |
| 0.4055 | 49.5935 | 2.4242 | 45 | Ca4ZrGe3O12 | 10.1039/d1qm01540k |
| 0.416154 | 74.11004 | 1.942885 | 10 | LiGe2(PO4)3 | 10.1016/j.jallcom.2022.163945 |
| 0.46375 | 45.42019 | 2.6575 | 40 | Sr3Sc4O9 | 10.1016/j.jallcom.2022.16458 |
| 0.228077 | 47.06008 | 1.832385 | 30 | Sc(PO3)3 | 10.1111/jace.18319 |
| 0.368571 | 47.07486 | 2.217357 | 40 | BaZrGe3O9 | 10.1016/j.jlumin.2021.118084 |
| 0.3553 | 45.8375 | 2.1342 | 66 | Ca2Lu1 Zr2Al3O12 | 10.1002/adom.201901684 |
| 0.3823 | 43.06635 | 2.1448 | 68 | La3Sc2Ga3O12 | 10.1016/j.jlumin.2018.05.076 |
| 0.327 | 45.0757 | 2.03715 | 86 | Y2Ca1Al4Si1O12 | 10.1039/C9TC05775G |
| 0.3543 | 45.8687 | 2.1255 | 60 | Ca2LuHf2Al3O12 | 10.1002/adom.201900185 |

| | | | | | |
|---|---|---|---|---|---|
| 0.3445 | 48.2613 | 2.28685 | 50 | Ca3Sc2Si3O12 | 10.1016/j.ceramint.2019.04.133 |
| 0.36285 | 45.7631 | 2.16505 | 60 | Ca2LaHf2Al3O12 | 10.1039/d0dt03840g |
| 0.35625 | 45.8302 | 2.1439 | 80 | Ca2YHf2Al3O12 | 10.1039/d0tc05657j |
| 0.3753 | 47.0065 | 2.1985 | 59 | Ca2LuScGa2Ge2O12 | 10.1021/acs.inorgchem.0c01890 |
| 0.34914 | 43.79806 | 1.9997 | 75 | Gd2.4Lu0.6Ga4AlO12 | 10.1016/j.cej.2021.132003 |
| 0.3281 | 50.8467 | 2.10095 | 70 | CaLu2Mg2Si3O12 | 10.1002/adom.202100388 |
| 0.36295 | 43.3899 | 2.05915 | 86 | Gd3ScAlGa3O12 | |
| 0.33375 | 48.9918 | 2.0549 | 84.2 | Y3Mg2AlSi2O12 | |
| 0.35595 | 46.2161 | 2.0741 | 63 | Gd3ScMgGa2SiO12 | |
| 0.36195 | 46.4376 | 2.0452 | 78 | Gd3MgAlGa2GeO12 | |
| 0.3767 | 49.20765 | 2.09425 | 51 | Gd3Mg2GaGe2O12 | |

**Table S4**. Element features.

| No. | Features | Abbreviations | Calculation formula |
|---|---|---|---|
| 1 | polarizability | P | $avg\ \bar{f} = \sum f_i x_i$ |
| 2 | ionic radius (shannon) | IR | |
| 3 | modulus rigidity | Mr | |
| 4 | thermal conductivity | Tc | |
| 5 | covalent radii | CR | |
| 6 | first ionization energy | FIE | |
| 7 | second ionization energy | SIE | |
| 8 | third ionization energy | TIE | |
| 9 | electronic affinity | AE | |
| 10 | fusion enthalpy | Hf | |
| 11 | cohesive energy (Brewer) | CEB | |
| 12 | valence electron number | VEC | |
| 13 | periodic number | Pn | |
| 14 | modulus bulk | Mb | |
| 15 | atomic volume(villars,daams) | Va | |
| 16 | atomic weight(villars,daams) | Ar | |
| 17 | molar volume | Mv | |
| 18 | electronegativity (martynov&batsanov) | En | |

**Table S5**. Spectroscopic parameters of $LnA_mB_{2-m}O_6$: $Cr^{3+}$ phosphor.

| Materials | λex (nm) | λem (nm) | FWHM (nm) |
|---|---|---|---|
| $LaAl_{0.5}Sb_{1.5}O_6$: $Cr^{3+}$ | 437, 608 | 851 | 200 |
| $LaGa_{0.5}Sb_{1.5}O_6$: $Cr^{3+}$ | 445, 618 | 851 | 200 |
| $LaIn_{0.5}Sb_{1.5}O_6$: $Cr^{3+}$ | 451, 631 | 867 | 204 |
| $LaMg_{1/3}Sb_{5/3}O_6$: $Cr^{3+}$ | 445, 621 | 874 | 203 |
| $GdGa_{0.5}Sb_{1.5}O_6$: $Cr^{3+}$ | 446, 602 | 703, 780 | 175 |
| $GdAl_{0.5}Sb_{1.5}O_6$: $Cr^{3+}$ | 443, 599 | 703, 777 | 147 |
| $LaGaTeO_6$: $Cr^{3+}$ | 430, 598 | 717, 780 | 151 |
| $LaAlTeO_6$: $Cr^{3+}$ | 429, 581 | 722 | 105 |

**Table S6.** Atom positions of LGS:0.04$Cr^{3+}$.

| x | Atom | x | y | z | Multiplicity & Wyckoff | Occ | Uiso |
|---|---|---|---|---|---|---|---|
| 0.04 | La1 | 0 | 0 | 0 | 1 | 1 | 0.01169 |
| | Ga1 | 0.333333 | 0.666667 | 0.5 | 2 | 0.23 | 0.00412 |
| | Sb1 | 0.333333 | 0.666667 | 0.5 | 2 | 0.75 | 0.00412 |
| | O1 | 0.368657 | 0 | 0.263036 | 6 | 1 | 0.00169 |
| | Cr1 | 0.333333 | 0.666667 | 0.5 | 2 | 0.02 | 0.00412 |

**Table S7**. Measured element ratios of LGS: 0.04$Cr^{3+}$.

| Element | La | O | Sb | Ga | Cr |
|---|---|---|---|---|---|
| Atom % | 12.23 | 63.45 | 18.49 | 5.16 | 0.67 |

**Calculation of Dq/B, Equation S1:**

$$10 \cdot D_q = E_a(^4T_{2g})$$

$$\frac{D_q}{B} = \frac{15 \cdot (x-8)}{x^2 - 10 \cdot x}$$

$$D_q \cdot x = E_a(^4T_{1g}) - E_a(^4T_{2g}) \quad \text{(S1)}$$

where $E_a(^4T_{1g})$ and $E_a(^4T_{2g})$ stand for the energy positions of $^4T_{1g}$ and $^4T_{2g}$. The relationship between Stokes shift and bandwidth was also considered, and $E_a(^4T_{2g})$ was determined as the average of the peak energies of the $^4A_{2g} \rightarrow {}^4T_{2g}$ excitation band and $^4T_{2g} \rightarrow {}^4A_{2g}$ emission band in this work.

**Calculation of activation energy, Equation S2:**

$$I_T = \frac{I_0}{1 + Cexp(-\Delta E/kT)} \quad \text{(S2)}$$

where $I_T$ is the emission intensity of the sample at temperature T, $I_0$ is the initial emission intensity, k represents the Boltzmann constant ($8.617 \times 10^{-5}$ eV $K^{-1}$) , and C is a constant. $\Delta E$ is the activation energy, which can be obtained by linearly fitting $ln(I_0/I_T)$ with $1/KT$.