Accelerated search for perovskite materials with higher Curie temperature based on the machine learning methods

/Supplementary information/

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Tab S1 the dataset for modeling

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NO. | molecular | ***Tc*** | ref | ***Ra*** | ***Rb*** | ***χpa*** | ***χpb*** | ***t*** | ***aO3*** | ***rc*** | ***I1a*** | ***I1b*** | ***Ra/Rb*** | ***M*** | ***EAa*** | ***EAb*** | ***tma*** | ***tmb*** | ***ta*** | ***tb*** | ***ΔfusHa*** | ***ΔfusHb*** | ***ρa*** | ***ρb*** |
| 1 | La0.7Sr0.3 Mn0.5Cr0.5O3 | 226 | [1] | 1.075 | 0.6 | 1.055 | 1.605 | 0.875 | 143.9 | 75.38 | 5.612 | 7.100 | 1.792 | 224.986 | 24.9 | 32.15 | 875.7 | 1576.5 | 2839.4 | 2366 | 56.66 | 319.5 | 5.097 | 7.23 |
| 2 | La0.7Sr0.3 Mn0.8Cr0.2O3 | 286 | [1] | 1.075 | 0.588 | 1.055 | 1.572 | 0.88 | 141.3 | 74 | 5.612 | 7.301 | 1.828 | 225.868 | 24.9 | 12.86 | 875.7 | 1378.2 | 2839.4 | 2183 | 56.66 | 268.8 | 5.097 | 7.27 |
| 3 | La0.7Sr0.3 Mn0.9Cu0.1O3 | 350 | [1] | 1.075 | 0.579 | 1.055 | 1.585 | 0.884 | 139.4 | 73.01 | 5.612 | 7.463 | 1.857 | 227.317 | 24.9 | 11.18 | 875.7 | 1229.9 | 2839.4 | 2111 | 56.66 | 231.85 | 5.097 | 7.47 |
| 4 | La0.75Sr0.25 MnO3 | 340 | [1] | 1.068 | 0.58 | 1.063 | 1.55 | 0.881 | 139.7 | 73.13 | 5.606 | 7.434 | 1.841 | 229.02 | 28.75 | 0 | 882.8 | 1246 | 2943.5 | 2061 | 54.65 | 235 | 5.273 | 7.30 |
| 5 | La0.7Sr0.3 Mn0.6Cr0.4O3 | 242 | [1] | 1.075 | 0.596 | 1.055 | 1.594 | 0.877 | 143 | 74.88 | 5.612 | 7.167 | 1.804 | 225.28 | 24.9 | 25.72 | 875.7 | 1510.4 | 2839.4 | 2305 | 56.66 | 302.6 | 5.097 | 7.24 |
| 6 | La0.7Sr0.25Ag0.05MnO3 | 303 | [2] | 1.074 | 0.58 | 1.104 | 1.55 | 0.883 | 139.7 | 73.13 | 5.706 | 7.434 | 1.851 | 227.47 | 32.63 | 0 | 884.9 | 1246 | 2878.4 | 2061 | 57.65 | 235 | 5.49 | 7.30 |
| 7 | La0.7Sr0.05Ag0.25MnO3 | 363 | [2] | 1.068 | 0.58 | 1.3 | 1.55 | 0.881 | 139.7 | 73.13 | 6.083 | 7.434 | 1.841 | 231.526 | 63.55 | 0 | 921.9 | 1246 | 3034.4 | 2061 | 61.61 | 235 | 7.062 | 7.30 |
| 8 | La0.75Ba0.1Ag0.15MnO3 | 315 | [3] | 1.08 | 0.58 | 1.204 | 1.55 | 0.886 | 139.7 | 73.13 | 5.841 | 7.434 | 1.862 | 237.03 | 51.94 | 0 | 905.5 | 1246 | 3110.2 | 2061 | 54.32 | 235 | 6.550 | 7.30 |
| 9 | La0.7Ca0.3MnO3 | 250 | [4] | 1.021 | 0.58 | 1.07 | 1.55 | 0.865 | 139.6 | 73.14 | 5.738 | 7.434 | 1.760 | 212.194 | 24.9 | 0 | 895.2 | 1246 | 2870 | 2061 | 95.15 | 235 | 4.767 | 7.30 |
| 10 | La0.7Ag0.3MnO3 | 270 | [4] | 1.066 | 0.58 | 1.349 | 1.55 | 0.881 | 139.7 | 73.13 | 6.177 | 7.434 | 1.838 | 232.54 | 71.28 | 0 | 931.1 | 1246 | 3073.4 | 2061 | 62.6 | 235 | 7.455 | 7.30 |
| 11 | La0.89Sr0.11MnO3 | 195 | [5] | 1.047 | 0.58 | 1.084 | 1.55 | 0.874 | 139.6 | 73.14 | 5.589 | 7.434 | 1.804 | 236.199 | 39.53 | 0 | 902.5 | 1246 | 3235.0 | 2061 | 49.022 | 235 | 5.764 | 7.30 |
| 12 | La0.88Sr0.12MnO3 | 170 | [5] | 1.048 | 0.58 | 1.082 | 1.55 | 0.874 | 139.6 | 73.14 | 5.591 | 7.434 | 1.807 | 235.686 | 38.76 | 0 | 901.1 | 1246 | 3214.2 | 2061 | 49.424 | 235 | 5.729 | 7.30 |
| 13 | La0.875Sr0.125MnO3 | 188 | [5] | 1.049 | 0.58 | 1.081 | 1.55 | 0.875 | 139.6 | 73.14 | 5.592 | 7.434 | 1.808 | 235.43 | 38.375 | 0 | 900.4 | 1246 | 3203.8 | 2061 | 49.625 | 235 | 5.711 | 7.30 |
| 14 | La0.865Sr0.135MnO3 | 214 | [5] | 1.05 | 0.58 | 1.080 | 1.55 | 0.875 | 139.6 | 73.14 | 5.593 | 7.434 | 1.811 | 234.917 | 37.605 | 0 | 899.0 | 1246 | 3182.9 | 2061 | 50.027 | 235 | 5.676 | 7.30 |
| 15 | La0.855Sr0.145MnO3 | 230.5 | [5] | 1.052 | 0.58 | 1.078 | 1.55 | 0.876 | 139.6 | 73.14 | 5.594 | 7.434 | 1.813 | 234.404 | 36.835 | 0 | 897.6 | 1246 | 3162.1 | 2061 | 50.429 | 235 | 5.641 | 7.30 |
| 16 | La0.845Sr0.155MnO3 | 242 | [5] | 1.053 | 0.58 | 1.077 | 1.55 | 0.876 | 139.6 | 73.14 | 5.595 | 7.434 | 1.816 | 233.892 | 36.065 | 0 | 896.1 | 1246 | 3141.3 | 2061 | 50.831 | 235 | 5.606 | 7.30 |
| 17 | La0.835Sr0.165MnO3 | 260.5 | [5] | 1.055 | 0.58 | 1.075 | 1.55 | 0.877 | 139.6 | 73.14 | 5.596 | 7.434 | 1.819 | 233.379 | 35.295 | 0 | 894.7 | 1246 | 3120.5 | 2061 | 51.233 | 235 | 5.571 | 7.30 |
| 18 | La0.83Sr0.17MnO3 | 265 | [5] | 1.056 | 0.58 | 1.075 | 1.55 | 0.877 | 139.6 | 73.14 | 5.597 | 7.434 | 1.820 | 233.122 | 34.91 | 0 | 894.0 | 1246 | 3110.1 | 2061 | 51.434 | 235 | 5.553 | 7.30 |
| 19 | La0.825Sr0.175 MnO3 | 283 | [5] | 1.056 | 0.58 | 1.074 | 1.55 | 0.877 | 139.6 | 73.14 | 5.598 | 7.434 | 1.821 | 232.866 | 34.525 | 0 | 893.3 | 1246 | 3099.7 | 2061 | 51.635 | 235 | 5.536 | 7.30 |
| 20 | La0.72Sr0.28MnO3 | 375 | [5] | 1.072 | 0.58 | 1.058 | 1.55 | 0.883 | 139.7 | 73.13 | 5.610 | 7.434 | 1.848 | 227.482 | 26.44 | 0 | 878.5 | 1246 | 2881.0 | 2061 | 55.856 | 235 | 5.167 | 7.30 |
| 21 | La0.69Sr0.31MnO3 | 380 | [5] | 1.077 | 0.58 | 1.054 | 1.55 | 0.884 | 139.7 | 73.13 | 5.613 | 7.434 | 1.856 | 225.943 | 24.13 | 0 | 874.3 | 1246 | 2818.6 | 2061 | 57.062 | 235 | 5.062 | 7.30 |
| 22 | La0.64Sr0.36MnO3 | 372 | [5] | 1.084 | 0.58 | 1.046 | 1.55 | 0.887 | 139.7 | 73.13 | 5.619 | 7.434 | 1.869 | 223.379 | 20.28 | 0 | 867.2 | 1246 | 2714.5 | 2061 | 59.072 | 235 | 4.886 | 7.30 |
| 23 | La0.52Sr0.48MnO3 | 330 | [5] | 1.102 | 0.58 | 1.028 | 1.55 | 0.894 | 139.7 | 73.12 | 5.634 | 7.434 | 1.900 | 217.226 | 11.04 | 0 | 850.3 | 1246 | 2464.6 | 2061 | 63.896 | 235 | 4.465 | 7.30 |
| 24 | La0.50Sr0.50MnO3 | 310 | [5] | 1.105 | 0.58 | 1.025 | 1.55 | 0.895 | 139.7 | 73.12 | 5.636 | 7.434 | 1.905 | 216.2 | 9.5 | 0 | 847.5 | 1246 | 2423 | 2061 | 64.7 | 235 | 4.395 | 7.30 |
| 25 | La0.48Sr0.52MnO3 | 290 | [5] | 1.108 | 0.58 | 1.022 | 1.55 | 0.896 | 139.7 | 73.12 | 5.638 | 7.434 | 1.910 | 215.174 | 7.96 | 0 | 844.7 | 1246 | 2381.4 | 2061 | 65.504 | 235 | 4.325 | 7.30 |
| 26 | La0.45Sr0.55MnO3 | 260 | [5] | 1.113 | 0.58 | 1.018 | 1.55 | 0.897 | 139.7 | 73.12 | 5.642 | 7.434 | 1.918 | 213.636 | 5.65 | 0 | 840.5 | 1246 | 2318.9 | 2061 | 66.71 | 235 | 4.220 | 7.30 |
| 27 | La0.4Sm0.3Sr0.3MnO3 | 256 | [6] | 1.054 | 0.58 | 1.076 | 1.55 | 0.876 | 139.6 | 73.14 | 5.632 | 7.434 | 1.817 | 229.906 | 24.6 | 0 | 922.5 | 1246 | 2338.4 | 2061 | 60.47 | 235 | 5.508 | 7.30 |
| 28 | Ba0.95Sr0.05MnO3 | 353 | [6] | 1.342 | 0.58 | 0.893 | 1.55 | 0.979 | 139.9 | 73.05 | 5.236 | 7.434 | 2.313 | 237.756 | -29 | 0 | 729.5 | 1246 | 1854.2 | 2061 | 53.45 | 235 | 3.571 | 7.30 |
| 29 | La0.7Sr0.3Mn0.93Fe0.07O3 | 296 | [7] | 1.075 | 0.578 | 1.055 | 1.567 | 0.885 | 139.2 | 72.88 | 5.612 | 7.467 | 1.860 | 226.520 | 24.9 | 1.099 | 875.7 | 1266.4 | 2839.4 | 2117 | 56.66 | 235.86 | 5.097 | 7.34 |
| 30 | La0.7Sr0.3Mn0.9Al0.1O3 | 310 | [7] | 1.075 | 0.576 | 1.055 | 1.556 | 0.886 | 138.5 | 72.51 | 5.612 | 7.290 | 1.866 | 223.66 | 24.9 | 4.26 | 875.7 | 1187.4 | 2839.4 | 2106.8 | 56.66 | 251.49 | 5.097 | 6.84 |
| 31 | La0.67Ca0.33Mn0.85V0.15O3 | 287.2 | [7] | 1.02 | 0.589 | 1.067 | 1.562 | 0.86 | 141.7 | 74.27 | 5.754 | 7.331 | 1.732 | 208.629 | 22.59 | 7.605 | 892.9 | 1345.6 | 2810.6 | 2262.9 | 100.205 | 263.05 | 4.629 | 7.11 |
| 32 | La0.57Nd0.1Sr0.23MnO3 | 339 | [7] | 0.957 | 0.58 | 0.960 | 1.55 | 0.842 | 139.6 | 73.16 | 5.041 | 7.434 | 1.649 | 216.686 | 25.39 | 0 | 804.1 | 1246 | 2599.7 | 2061 | 49.876 | 235 | 4.814 | 7.30 |
| 33 | La0.6Nd0.1Ca0.15Sr0.15Mn0.9Fe0.1O3 | 298 | [7] | 1.043 | 0.577 | 1.067 | 1.578 | 0.874 | 138.9 | 72.76 | 5.670 | 7.481 | 1.808 | 219.946 | 24.8 | 1.57 | 895.8 | 1275.2 | 2815.7 | 2141 | 76.395 | 236.23 | 5.018 | 7.36 |
| 34 | La0.6Nd0.1Ca0.15Sr0.15Mn0.95Fe0.05O3 | 306 | [7] | 1.043 | 0.579 | 1.067 | 1.564 | 0.873 | 139.4 | 73.01 | 5.670 | 7.457 | 1.803 | 219.901 | 24.8 | 0.785 | 895.8 | 1260.6 | 2815.7 | 2101 | 76.395 | 235.62 | 5.018 | 7.33 |
| 35 | La0.6Nd0.1Ca0.15Sr0.15MnO3 | 326 | [7] | 1.043 | 0.58 | 1.067 | 1.55 | 0.872 | 139.6 | 73.14 | 5.670 | 7.434 | 1.798 | 219.855 | 24.8 | 0 | 895.8 | 1246 | 2815.7 | 2061 | 76.395 | 235 | 5.018 | 7.30 |
| 36 | La0.9Pb0.1MnO3 | 235 | [8] | 1.005 | 0.58 | 1.177 | 1.55 | 0.859 | 139.6 | 73.15 | 5.761 | 7.434 | 1.733 | 248.67 | 46.71 | 0 | 858.9 | 1246 | 3292.5 | 2061 | 42.45 | 235 | 6.665 | 7.30 |
| 37 | La0.8Pb0.2MnO3 | 310 | [8] | 0.98 | 0.58 | 1.254 | 1.55 | 0.85 | 139.6 | 73.15 | 5.945 | 7.434 | 1.690 | 255.5 | 45.42 | 0 | 799.9 | 1246 | 3121 | 2061 | 40.3 | 235 | 7.18 | 7.30 |
| 38 | La0.7Pb0.3MnO3 | 358 | [8] | 0.955 | 0.58 | 1.331 | 1.55 | 0.841 | 139.6 | 73.16 | 6.129 | 7.434 | 1.647 | 262.33 | 44.13 | 0 | 740.8 | 1246 | 2949.5 | 2061 | 38.15 | 235 | 7.695 | 7.30 |
| 39 | La0.6Pb0.4MnO3 | 360 | [8] | 0.93 | 0.58 | 1.408 | 1.55 | 0.832 | 139.5 | 73.16 | 6.313 | 7.434 | 1.603 | 269.16 | 42.84 | 0 | 681.8 | 1246 | 2778 | 2061 | 36 | 235 | 8.21 | 7.30 |
| 40 | La0.5Pb0.5MnO3 | 355 | [8] | 0.905 | 0.58 | 1.485 | 1.55 | 0.823 | 139.5 | 73.17 | 6.497 | 7.434 | 1.560 | 275.99 | 41.55 | 0 | 622.7 | 1246 | 2606.5 | 2061 | 33.85 | 235 | 8.725 | 7.30 |
| 41 | La0.65Sr0.35MnO3 | 377 | [9] | 1.083 | 0.58 | 1.048 | 1.55 | 0.887 | 139.7 | 73.13 | 5.618 | 7.434 | 1.866 | 223.892 | 21.05 | 0 | 868.7 | 1246 | 2735.3 | 2061 | 58.67 | 235 | 4.922 | 7.30 |
| 42 | La0.55Pr0.1Sr0.35MnO3 | 353 | [9] | 1.079 | 0.58 | 1.051 | 1.55 | 0.885 | 139.7 | 73.13 | 5.608 | 7.434 | 1.859 | 224.092 | 20.95 | 0 | 869.9 | 1246 | 2740.9 | 2061 | 59.1 | 235 | 4.984 | 7.30 |
| 43 | La0.45Pr0.2Sr0.35MnO3 | 344 | [9] | 1.075 | 0.58 | 1.054 | 1.55 | 0.884 | 139.7 | 73.13 | 5.597 | 7.434 | 1.853 | 224.292 | 20.85 | 0 | 871.3 | 1246 | 2746.5 | 2061 | 59.53 | 235 | 5.046 | 7.30 |
| 44 | La0.35Pr0.3Sr0.35MnO3 | 334 | [9] | 1.071 | 0.58 | 1.057 | 1.55 | 0.882 | 139.7 | 73.13 | 5.587 | 7.434 | 1.846 | 224.492 | 20.75 | 0 | 872.6 | 1246 | 2752.1 | 2061 | 59.96 | 235 | 5.108 | 7.30 |
| 45 | La0.7Sr0.1Ag0.2 MnO3 | 286.5 | [4] | 1.069 | 0.58 | 1.251 | 1.55 | 0.882 | 139.7 | 73.13 | 5.989 | 7.434 | 1.843 | 230.512 | 55.82 | 0 | 912.7 | 1246 | 2995.4 | 2061 | 60.62 | 235 | 6.669 | 7.30 |
| 46 | La0.67Sr0.33MnO3 | 372.5 | [5] | 1.08 | 0.58 | 1.051 | 1.55 | 0.885 | 139.7 | 73.13 | 5.616 | 7.434 | 1.861 | 224.918 | 22.59 | 0 | 871.5 | 1246 | 2776.9 | 2061 | 57.866 | 235 | 4.992 | 7.30 |
| 47 | La0.7Sr0.3MnO3 | 370 | [5] | 1.075 | 0.58 | 1.055 | 1.55 | 0.884 | 139.7 | 73.13 | 5.612 | 7.434 | 1.853 | 226.456 | 24.9 | 0 | 875.7 | 1246 | 2839.4 | 2061 | 56.66 | 235 | 5.097 | 7.30 |

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Steps to follow:

1. First copy and paste the data set above in Excel
2. Transform/change to data from Tab S1 into csv format
3. Use the data set and read it in Matlab
4. Use the data set as an input data set to the code/in the code Gradient descent applied to RBFNNs (I have already shared this with in previous tutorial)
5. The type of result you will produce by running the code is the training Root-Mean-Square-Error (RMSE) and compare to the value obtained in Table 5 from article:

**Accelerated search for perovskite materials with higher Curie temperature based on the machine learning methods**

1. Fill the supervision form explained during the supervision form.