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# Correlation selection of perovskites with optimal parameters

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## ABSTRACT

A descriptor is constructed to predict the composition of $ABO_3$ perovskites that do not contain transition metals and have a high level of ionic conductivity (σ). The descriptor consists of two parts: the ratio of ionic radii, RA/RB and the ratio of ionization potentials, VB/VA for A- and B- cations. Parameters for 100 perovskite compounds were considered to find the correlation dependences between the descriptor and the magnitude ofσ. Correlation selection approach is proposed to reveal a suitable correlation series. This approach allows determining the composition of perovskites that has a desirable ionic conductivity. 

**Keywords:** Perovskites; ionic transport; non-transition metals.

## Introduction

Perovskites have been intensively studied due to their numerous applications today and wide perspectives of new applications in future [**1-5**]. Service characteristics, physical and chemical properties of these materials are extremely sensitive to their composition. Even slightest changes of composition of perovskites dramatically alter their properties. Therefore the improvement and modification of these materials require a long and work-consuming experimental and theoretical search. *Ab initio* calculations [**6-10**], and also semi-empirical methods (see, for example, [**11**]) are used to predict the best parameters of perovskites.

In [**12**] the descriptor based on the parameters of electronic structure of perovskite compounds was proposed and calculated to optimize the oxygen reduction reaction (ORR) in SOFC cathodes. This descriptor was determined as the position of center of the oxygen *p*-band calculated with respect to Fermi energy. It was found that this descriptor correlates well with the overall ORR activity. However, the calculation of this descriptor is considerably time-consuming.

As a rule the semi-empirical methods lead faster to practically useful results. The most well-known semi-empirical approaches are based on concepts of Goldschmidt tolerance factor [**13**], critical radius and lattice free volume [**14, 15**], Pauling rules [**16**]. In all these cases either geometric or energy-based empirical parameters are used. The choice of the descriptor is dictated by the necessity of the strong sensitivity of considered properties of material with respect to the parameters that are chosen for the construction of a descriptor.

Authors of [**17**] obtained criteria for the improvement of the formability of perovskite-type oxides using a structure-map technology. The map is based on two geometric parameters: octahedral factor ($R_B/R_O$) and tolerance factor *t* [**18**] ($R_B$ and $R_O$ are ionic radii of B – atom and Oxygen atom in the perovskite lattice). The model was developed considering 173 $ABO_3$ compounds. It was found that the octahedral factor is as important as the tolerance factor [**18**] with regards to the formability of perovskite type oxides.

Series of works were directed to find the so-called Global Instability Index (GII) [**19**]. Authors of [**20**] applied the artificial neural networks (ANNs) modelling to predict GII. They showed a significant role of the bond-valence tolerance factor $t_{BV}$ [**21**] in the determination of GII. Earlier the application of ANNs modelling to predict structural stability and formability of $ABO_3$ - type perovskites was realized in [**22**].

There are strong experimental evidences concerning the dependence of the structural stability of perovskites on the sizes of their constituent atoms. Authors of [**23**] studied $R_2BaCuO_5$ compounds, with R = rare earth atom from Sm to Lu, by neutron and X-ray powder diffraction. A systematic variation of structural stability was found depending on the size of the rare earth atom.

The above mentioned and others results [**24,25**] show that the geometric factors as well as the energy characteristics of crystal can be used to construct the appropriate descriptor for prediction of a structural stability or a formability of perovskites. In this context we would like to note two points. The first one is that in most cases the simultaneous use of geometric and energy parameters for the construction of descriptor are almost no found. The second one is that the constructed descriptors are mainly aimed to predict the structural stability or the formability of

 

perovskites but not their physical and service characteristics.

In [**26**] we described an approach for the search of $ABO_3$ perovskites with high rates of ionic transport. The ionic transport in perovskites with transition metals (TM) at B – site was considered in terms of the theory of coordination compounds. The stability of these materials is sensitive to the values of the effective charge of the ions of TM ($Z^*$) and to the electronegativity ($\chi$) of the surrounding cations (ligands). This is because the stability is determined by the splitting parameter $\Delta$ for degenerated *d*-levels, which in turn is proportional to $Z^* \cdot \chi$. Thus the transition element determine to considerable extent the stability of perovskite lattice and hence the processes of defect formation including the formation of vacancies.

On the basis of these considerations the descriptor for the ionic transport rate in perovskites with TM was defined as product $Z^* \cdot \chi$.

At the same time the perovskites with only non-transition elements also exhibit useful properties such as, for example, a high ionic conductivity. Analysis of published works showed that in this case the energy characteristics of valence electrons of cations at both A and B sites determine the bonding and stability of perovskites. For some compounds the promotion of *s*-and *p*-electrons to *d*-states occurs. For example, this effect is observed in perovskites, which include Bismuth. These perovskites attract attention due to their wide practically important applications [**27-32**]. In [**27, 31**] a theoretical model is presented for electronic structure of $BaBiO_3$ compound. By treating two types of Bi with different electron configurations ($6s^26p^36d^0$(I) and $7s^06p^36d^0$(II)), i.e. differently ionized Bi atoms, $Bi^{5+}$ and $Bi^{3+}$, and using LMTO-ASA approach total and partial densities of states for electrons were obtained for $Ba_4Bi_4O_{12}$ supercell [**31**]. The promotion of electrons to Bi (I)-6*d* and less pronounced promotion in the case of Bi (II)-6*d* was revealed. This example demonstrates that for perovskites with non-transition elements the stability of the lattice should be determined by the energy characteristics of *valence* electrons of cations *both* at A- and B- sites that are responsible for the bonding in these compounds. Keeping in mind the fact that atomic radii mismatch may lead to the decomposition of the solid solutions the geometry characteristics of these cations should be also included in consideration.

The earlier descriptor (based on effective charge and electronegativity) designed for $ABO_3$ type perovskites having transition metals at B site does not work for the $ABO_3$ materials with non-transition metals.

In the present work, unlike [**26**], we studied $ABO_3$ perovskites that contain only non-transition elements. A new descriptor that includes the ionization potentials for valence electrons of A and B cations and their ionic radii is constructed.

Applying this descriptor we found a good correlation for predicting the composition of compounds with high ionic conductivity.

**Table 1**. Parameters for the descriptor $\Delta$ and the ionic conductivity of perovskites ($R_A$ and $R_B$ are in pm, $V_A$ and $V_B$ are in eV).

| No | Compound | $R_A$ | $V_A$ | $R_B$ | $V_B$ | Log σ | $\Delta_1$ | $\Delta_2$ | $\Delta$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | $La_{0.9}Sr_{0.1}Ga_{0.9}Mg_{0.1}O_3$ | 195 | 802 | 134 | 1736.4 | -0.5[33] | 0.04 | 0.16 | 0.24 |
| 2 | $(La_{0.72}Nd_{0.08})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_3$ | 199 | 802 | 134 | 1736.4 | -0.6[34] | 0.02 | 0.16 | 0.2 |
| 3 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Co_{0.1}O_3$ | 184.5 | 794.6 | 125 | 1662.1 | -1.0[33] | 0.03 | 0.1 | 0.16 |
| 4 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Si_{0.1}O_3$ | 196 | 723.1 | 134 | 1417.6 | -1.0[33] | 0.04 | 0.04 | 0.12 |
| 5 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Be_{0.1}O_3$ | 196 | 750 | 133 | 1552.3 | -1.0[33] | 0.03 | 0.07 | 0.13 |
| 6 | $La_{0.9}Sr_{0.1}Ga_{0.8}Mg_{0.2}O_3$ | 195.5 | 803 | 134 | 1736.4 | -1.0[33] | 0.04 | 0.16 | 0.24 |
| 7 | $(La_{0.9}Nd_{0.1})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_3$ | 195.2 | 765.8 | 134 | 1656.4 | -1.1[34] | 0.04 | 0.16 | 0.24 |
| 8 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Zn_{0.1}O_3$ | 184.5 | 794.6 | 126 | 1673.6 | -1.2[33] | 0.04 | 0.11 | 0.23 |
| 9 | $(La_{0.9}Cd_{0.1})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_3$ | 194.8 | 762 | 134 | 1656.4 | -1.3[34] | 0.05 | 0.17 | 0.27 |
| 10 | $(La_{0.9}Y_{0.1})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_3$ | 194.8 | 753 | 134 | 1656.4 | -1.4[34] | 0.05 | 0.17 | 0.27 |
| 11 | $La_{0.9}Sr_{0.1}Ga_{0.9}In_{0.1}O_3$ | 195.5 | 823 | 132.5 | 1783.4 | -1.4[33] | 0.02 | 0.17 | 0.21 |
| 12 | $BaTb_{0.9}In_{0.1}O_3$ | 235 | 635 | 160 | 1127.3 | -1.4[33] | 0.03 | 0.23 | 0.29 |
| 13 | $Sm_{0.9}Ca_{0.1}AlO_3$ | 184.5 | 813.3 | 125 | 1813 | -1.5[35] | 0.02 | 0.23 | 0.27 |
| 14 | $Yb_{0.9}Ca_{0.1}AlO_3$ | 175.5 | 887 | 125 | 1713 | -1.5[35] | 0.1 | 0.07 | 0.27 |
| 15 | $Gd_{0.85}Ca_{0.15}AlO_3$ | 180 | 879.6 | 125 | 1713 | -1.5[36] | 0.06 | 0.05 | 0.23 |
| 16 | $(La_{0.9}Yb_{0.1})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_3$ | 194.4 | 767 | 134 | 1656.4 | -1.6[35] | 0.05 | 0.16 | 0.36 |
| 17 | $La_{0.9}Sr_{0.1}Ga_{0.9}In_{0.1}O_3$ | 195 | 813 | 133 | 1825.4 | -1.7[37] | 0.02 | 0.24 | 0.28 |
| 18 | $La_{0.8}Sr_{0.2}GaO_{2.9}$ | 196 | 803.4 | 130 | 1840 | -2.0[38] | 0.01 | 0.29 | 0.31 |
| 19 | $La_{0.9}Sr_{0.1}Sc_{0.9}Mg_{0.1}O_3$ | 195.5 | 803 | 140 | 1526.2 | -2.0[37] | 0.11 | 0.1 | 0.32 |
| 20 | $Nd_{0.9}Ca_{0.1}Al_{0.5}Ga_{0.5}$ | 184.5 | 794.6 | 127.5 | 1876.5 | -2.0[33] | 0.05 | 0.24 | 0.34 |
| 21 | $(La_{0.8}Sr_{0.2})(Ga_{0.8}Mg_{0.115}Co_{0.085})O_3$ | 196 | 803.4 | 135.5 | 1795.3 | -2.0[37] | 0.05 | 0.23 | 0.33 |
| 22 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Ni_{0.1}O_3$ | 184 | 784.6 | 128 | 1696.2 | -2.0[33] | 0.07 | 0.16 | 0.3 |
| 23 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Be_{0.1}O_3$ | 185.5 | 794.6 | 115 | 1674.5 | -2.0[33] | 0.11 | 0.11 | 0.33 |
| 24 | $La_{0.9}Sr_{0.1}GaO_3$ | 195.5 | 803 | 130 | 1840 | -2.0[38] | 0.01 | 0.29 | 0.31 |
| 25 | $La_{0.5}Sr_{0.5}Ga_{0.7}Zr_{0.3}O_{2.875}$ | 187.5 | 804 | 138.8 | 1574 | -2.0[39] | 0.15 | 0.08 | 0.38 |
| 26 | $La_{0.9}Sr_{0.1}InO_{2.95}$ | 195.5 | 803 | 145 | 1694 | -2.1[39] | 0.15 | 0.11 | 0.41 |
| 27 | $La_{0.9}Sr_{0.1}Ga_{0.9}Al_{0.1}O_3$ | 195.5 | 803 | 125 | 1825.3 | -2.1[33] | 0.06 | 0.27 | 0.39 |
| 28 | $La_{0.9}Sr_{0.1}Ga_{0.9}Mg_{0.1}O_3$ | 195.5 | 803 | 128 | 1788.2 | -2.1[33] | 0.06 | 0.23 | 0.35 |
| 29 | $Pr_{0.9}Ca_{0.1}AlO_3$ | 174.5 | 782.8 | 125 | 1713 | -2.1[40] | 0.11 | 0.19 | 0.41 |
| 30 | $La_{0.5}Sr_{0.5}Ga_{0.7}Zr_{0.3}O_{2.9}$ | 197.5 | 804 | 137.5 | 1826 | -2.1[39] | 0.06 | 0.27 | 0.39 |
| 31 | $La_{0.5}Sr_{0.5}Ga_{0.75}Zr_{0.25}O_{2.925}$ | 197.5 | 804 | 139 | 1788 | -2.1[39] | 0.08 | 0.15 | 0.31 |
| 32 | $BaZr_{0.3}In_{0.7}O_3$ | 215 | 712.6 | 155 | 1492.3 | -2.1[39] | 0.11 | 0.09 | 0.31 |
| 33 | $BaZr_{0.5}In_{0.5}O_{2.75}$ | 215 | 732.6 | 155 | 1324 | -2,2[39] | 0.11 | 0.2 | 0.35 |
| 34 | $BaIn_{0.9}Ca_{0.1}O_3$ | 215 | 732.6 | 135.5 | 1611,3 | -2.3[39] | 0.09 | 0.2 | 0.38 |
| 35 | $CaCe_{0.9}Er_{0.1}O_3$ | 174.5 | 867.6 | 125.5 | 1611.5 | -2.3[33] | 0.11 | 0.14 | 0.36 |
| 36 | $BaZr_{0.1}In_{0.9}O_3$ | 215 | 732.6 | 155 | 1620 | -2.4[39] | 0.11 | 0.21 | 0.43 |
| 37 | $BaZr_{0.4}In_{0.6}O_3$ | 215 | 742.6 | 155 | 1398 | -2.4[39] | 0.11 | 0.12 | 0.36 |
| 38 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Ga_{0.1}O_3$ | 174.5 | 734.6 | 125 | 1725.7 | -2.4[41] | 0.1 | 0.35 | 0.45 |
| 39 | $Nd_{0.9}Ca_{0.1}Ga_3O_3$ | 180 | 794.6 | 125 | 1840 | -2.4[41] | 0.06 | 0.32 | 0.44 |
| 40 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Cu_{0.1}$ | 184.5 | 794.6 | 136 | 1696.8 | -2.4[42] | 0.15 | 0.14 | 0.44 |
| 41 | $Na_{0.9}Ca_{0.1}Al_{0.5}Ga_{0.5}O_3$ | 180 | 763.2 | 127.5 | 1726.5 | -2.4[43] | 0.09 | 0.26 | 0.44 |
| 42 | $BaCe_{1-y}Y_yO_3$ | 215 | 735 | 154 | 1296.6 | -2.4[39] | 0.1 | 0.24 | 0.44 |
| 43 | $SrTi_{0.9}Al_{0.1}O_3$ | 185 | 955 | 138.5 | 1711 | -2.5[40] | 0.16 | 0.21 | 0.52 |
| 44 | $La_{0.9}Sr_{0.1}In_{0.9}Mg_{0.1}O_3$ | 195.5 | 803 | 145.5 | 1716.8 | -2.5[39] | 0.16 | 0.14 | 0.46 |
| 45 | $Na_{0.9}Ca_{0.1}Al_{0.7}Ga_{0.3}O_3$ | 180 | 753.2 | 126.5 | 1751.1 | -2.6[41] | 0.08 | 0.32 | 0.48 |
| 46 | $Na_{0.9}Ca_{0.1}Al_{0.2}Ga_{0.8}O_3$ | 180 | 733.2 | 129 | 1714 | -2.6[41] | 0.1 | 0.34 | 0.44 |
| 47 | $La_{0.9}Sr_{0.1}AlO_{2.95}$ | 195.5 | 800 | 125 | 1890 | -2.6[33] | 0.06 | 0.36 | 0.48 |
| 48 | $La_{0.9}Ca_{0.1}GaO_{2.95}$ | 193.5 | 739 | 130 | 1840 | -2.7[33] | 0.01 | 0.49 | 0.51 |
| 49 | $Ba_3In_2CeO_8$ | 197 | 795.6 | 125 | 1840 | -2.7[33] | 0.08 | 0.31 | 0.47 |
| 50 | $Nd_{0.9}Sr_{0.1}GaO_3$ | 196 | 832.6 | 135 | 1840 | -2.7[39] | 0.15 | 0.2 | 0.5 |
| 51 | $NdGa_{0.9}Mg_{0.1}O_3$ | 185 | 786.5 | 132 | 1848,2 | -2.7[44] | 0.1 | 0.34 | 0.54 |
| 52 | $BaZr_{0.2}In_{0.8}O_3$ | 215 | 732.6 | 155 | 1746 | -2.7[45] | 0.11 | 0.38 | 0.5 |
| 53 | $BaCe_{(1-z-y)}Zr_zY_yO_3$ | 215 | 732 | 159 | 1288 | -2.8[45] | 0.15 | 0.25 | 0.55 |
| 54 | $BaCe_{(1-z-y-p)}Zr_zY_yPr_pO_3$ | 215 | 735 | 159 | 1288.4 | -2.8[45] | 0.15 | 0.25 | 0.55 |
| 55 | $Na_{0.9}Ca_{0.1}AlO_3$ | 180 | 733 | 125 | 1770 | -2.8[44] | 0.06 | 0.41 | 0.53 |
| 56 | $Na_{0.9}Ca_{0.1}Al_{0.8}Ga_{0.2}O_3$ | 180 | 733.2 | 126 | 1750.4 | -2.9[45] | 0.07 | 0.39 | 0.53 |
| 57 | $Nd_{0.9}Ca_{0.1}AlO_{2.95}$ | 184 | 784 | 128 | 1893 | -2.9[39] | 0.06 | 0.41 | 0.53 |
| 58 | $La_{0.5}Sr_{0.5}Ga_{0.6}Zr_{0.4}O_{2.95}$ | 197.5 | 804 | 145 | 1388.2 | -2.9[39] | 0.14 | 0.27 | 0.56 |
| 59 | $Nd_{0.9}Ca_{0.9}Al_{0.9}Be_{0.1}O_3$ | 195.5 | 803 | 115 | 1493 | -3.0[33] | 0.2 | 0.14 | 0.54 |
| 60 | $La_{0.9}Ba_{0.1}Al\ O_3$ | 197 | 705.6 | 125 | 1713 | -3.0[39] | 0.08 | 0.43 | 0.59 |
| 61 | $Sr_{0.9}Ba_{0.1}Sc_{0.6}Al_{0.3}Mg_{0.1}O_3$ | 197 | 800 | 145.5 | 1366 | -3.0[39] | 0.15 | 0.29 | 0.59 |
| 62 | $BaCe_{0.9}Gd_{0.1}O_3$ | 215 | 735 | 150.5 | 1140 | -3.0[46] | 0.07 | 0.45 | 0.59 |
| 63 | $SrSc_{0.65}Al_{0.35}\ Al_{0.5}O_{2.5}$ | 180 | 955 | 125 | 1477.5 | -3.0[39] | 0.06 | 0.45 | 0.57 |
| 64 | $BaZr_{0.7}In_{0.3}O_3$ | 215 | 746.6 | 155 | 1225 | -3.1[39] | 0.11 | 0.36 | 0.58 |
| 65 | $BaZr_{0.6}In_{0.4}O_3$ | 215 | 752.6 | 155 | 1217 | -3.1[39] | 0,11 | 0.38 | 0.6 |
| 66 | $Na_{0.9}Ca_{0.1}GaO_3$ | 180 | 753.2 | 133 | 1740 | -3.1[47] | 0.15 | 0.31 | 0.61 |
| 67 | $La_{0.9}Ca_{0.1}Al\ O_{2.95}$ | 193.5 | 725 | 125 | 1813 | -3.2[39] | 0.05 | 0.5 | 0.6 |
| 68 | $Sr_{0.9}Ba_{0.1}Sc_{0.6}Al_{0.4}Al0.5 \rightarrow O_{2.5}$ | 191 | 800 | 133 | 1245 | -3.2[39] | 0.07 | 0.45 | 0.59 |
| 69 | $La_{0.7}Ba_{0.3}Al\ O_3$ | 190.5 | 705.7 | 125 | 1813 | -3.3[47] | 0.02 | 0.57 | 0.61 |
| 70 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Mg_{0.1}O_3$ | 184 | 730.6 | 127.5 | 1822.4 | -3.4[33] | 0.06 | 0.49 | 0.61 |
| 71 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Zr_{0.1}O_3$ | 184 | 721 | 128 | 1801.2 | -3.4[39] | 0.06 | 0.49 | 0.61 |
| 72 | $Nd_{0.9}Sr_{0.1}AlO_{2.95}$ | 186.5 | 712.6 | 125 | 1866 | -3.4[39] | 0.01 | 0.62 | 0.64 |
| 73 | $SrSc_{0.6}Al_{0.4}\ Al_{0.5}O_{2.5}$ | 155 | 945 | 107 | 1369 | -3.4[39] | 0.05 | 0.55 | 0.65 |
| 74 | $SrSc_{0.5}Al_{0.4}\ Mg_{0.1}O_3$ | 165 | 945 | 113 | 1356 | -3.4[39] | 0.04 | 0.56 | 0.64 |
| 75 | $BaZr_{0.8}In_{0.2}O_3$ | 215 | 732.6 | 155 | 1148 | -3.5[39] | 0.11 | 0.43 | 0.65 |
| 76 | $Sr_2ScAl_{0.8}Zn_{0.2}O_{4.9}$ | 185 | 781.3 | 136 | 1840 | -3.6[39] | 0.14 | 0.36 | 0.64 |
| 77 | $Ni_{0.9}Ba_{0.1}GaO_{2.95}$ | 195.5 | 843 | 135 | 1220.3 | -3.6[39] | 0.05 | 0.55 | 0.65 |
| 78 | $La_{0.5}Sr_{0.5}Ga_{0.55}Zr_{0.45}O_3$ | 197.5 | 844 | 126.5 | 1248.4 | -3.7[39] | 0.06 | 0.52 | 0.64 |
| 79 | $SrSc_{0.5}Al_{0.4}\ Zn_{0.1}O_3$ | 155 | 955 | 108.5 | 1420 | -3.7[39] | 0.07 | 0.51 | 0.65 |
| 80 | $SrSc_{0.5}Al_{0.45}\ Mg_{0.05}O_3$ | 155 | 955 | 112.5 | 1533.5 | -3.8[39] | 0.13 | 0.39 | 0.65 |
| 81 | $SrSc_{0.5}Al_{0.35}\ Mg_{0.15}O_3$ | 155 | 955 | 109.5 | 1454.5 | -3.8[39] | 0.9 | 0.48 | 0.66 |
| 82 | $SrSc_{0.5}Al_{0.45}\ Zn_{0.05}O_3$ | 155 | 955 | 111 | 1488,9 | -3.8[39] | 0.11 | 0.44 | 0.66 |
| 83 | $SrSe_{0.5}Al_{0.45}Y_{0.05}Al_{0.5}O_{2.5}$ | 155 | 955 | 104.2 | 1498 | -3.8[39] | 0.11 | 0.43 | 0.65 |
| 84 | $SrSc_{0.5}Al_{0.4}Y_{0.1}Al_{0.5}O_{2.5}$ | 155 | 955 | 105 | 1350 | -3.8[39] | 0.03 | 0.59 | 0.65 |
| 85 | $Sr_{0.8}Ba_{0.2}Sc_{0.5}Al_{0.5}O_{2.5}$ | 203 | 798 | 143 | 1213 | -3.9[39] | 0.09 | 0.48 | 0.66 |
| 86 | $Nd_{0.9}Ca_{0.1}Al_{0.9}Si_{0.1}O_3$ | 183.5 | 753 | 128.5 | 1895.5 | -4.0[33] | 0.08 | 0.51 | 0.67 |
| 87 | $SrSc_{0.55}Al_{0.45}\ Al_{0.5}O_{2.5}$ | 225 | 955 | 144.2 | 1384.1 | -4.0[39] | 0.06 | 0.55 | 0.67 |
| 88 | $Nd_{0.9}Ba_{0.1}AlO_{2.95}$ | 188 | 721.3 | 120 | 1813 | -4.0[39] | 0.07 | 0.51 | 0.65 |
| 89 | $BaZr_{0.9}In_{0.1}O_{2.95}$ | 215 | 722.6 | 155 | 1129 | -4.1[39] | 0.06 | 0.44 | 0.66 |
| 90 | $Sr_{0.9}Ba_{0.1}Sc_{0.5}Al_{0.5}O_{2.5}$ | 191 | 800 | 143 | 1323 | -4.3[39] | 0.17 | 0.34 | 0.68 |
| 91 | $SrSe_{0.45}Y_{0.05}\ Al_{0.5}O_{2.5}$ | 155 | 955 | 134 | 1800.5 | -4.4[39] | 0.26 | 0.12 | 0.64 |
| 92 | $SrSc_{0.4}Y_{0.1}Al_{0.5}O_{2.5}$ | 175 | 955 | 135 | 1618 | -4.5[39] | 0.21 | 0.31 | 0.73 |
| 93 | $SrSc_{0.5}Al_{0.5}O_{2.5}$ | 175 | 935 | 142.5 | 1995 | -4.7[39] | 0.027 | 0.13 | 0.67 |
| 94 | $NdAlO_3$ | 170 | 766.5 | 130 | 1913 | -5.0[33] | 0.19 | 0.49 | 0.87 |
| 95 | $Cd_{0.9}Ca_{0.1}AlO_3$ | 175 | 988.5 | 135 | 1413 | -5.0[47] | 0.21 | 0.57 | 0.99 |
| 96 | $SrZrO_3$ | 200 | 806.8 | 155 | 1955 | -5.4[33] | 0.21 | 0.42 | 1.05 |
| 97 | $Y_{0.9}Ca_{0.1}AlO_3$ | 170 | 1689 | 125 | 1713 | -6.0[47] | 0.06 | 0.99 | 1.11 |
| 98 | $BaZnO3$ | 163.5 | 709 | 125 | 1913 | -6.0[39] | 0.19 | 0.69 | 1.07 |
| 99 | $BaZrO_3$ | 215 | 722.6 | 165 | 1955 | -6.1[39] | 0.2 | 0.7 | 1,10 |
| 100 | $BaCe_{(1-y-p)}Y_yPr_pO_3$ | 215 | 735 | 184 | 1099.4 | -7.0[45] | 0.33 | 0.5 | 1.16 |

## Experimental

*Goal seek of descriptor for perovskites with only non- transition metals*

The descriptor approach allows speeding up a creation of new materials with desired properties. The main requirements to descriptors are:

- A descriptor should be closely related with the property of interest;
- The descriptor changes and the changes of the material property should be well correlated;
- The above correlation should be kept for a certain interval of the material property changes;
- The calculations for the construction of descriptor should be as easy as possible.

In fact all geometry parameters in descriptors indirectly linked to energy characteristics of crystal. Interatomic distances linked to the bonding energy through the overlap integrals. Goldschmidt tolerance factor, critical radius and lattice free volume are determined indirectly by the parameters of the corresponding potentials of interatomic interaction.

In this work we propose a combined descriptor starting from the fact that in all cases the geometric parameters (sizes of A and B – cations, interatomic distances) as well as energy characteristics (ionization potentials of A and B – cations, parameters of band structure) in conjunction determine the perovskite properties. Constructing this descriptor we have chosen as the main parameters the ionic radii (RA and RB) and the mean potential of valence electrons (VA and VB) for cations A and B. In the case of mixed perovskites (if there is more than one A or B cations) the values of radii and potentials are taken as a weighted sum with the atomic fractions of constituents on the specific sites. For each cation the ionization potential is taken as the average for all electrons involved in the valence bonds. For predicting the composition of compounds with high level ionic conductivity (σ) we have constructed a descriptor containing two parts: the ratios RA/RB and VB/VA. Parameters for 100 perovskite compounds that were considered are presented in **Table 1**. The source for conductivity data is cited in the brackets in **Table 1**. The ionic radii and ionization potentials of the components of complex perovskites that are necessary to calculate RA, RB, VA and VB presented in **Table 1** are taken from [**48, 49**].

One can see that the largest values of ionic conductivity (σ) correspond to the cases when RA/RB=1.5 and VB/VA=2. We denote the deviations from these optimal values as: $\Delta_1$ and $\Delta_2$. $\Delta_1 = |1.5 - RA/RB|$; $\Delta_2 = |2 - VB/VA|$. The proposed descriptor is introduced as $\Delta = k\Delta_1 + \Delta_2$ where k is a fitting parameter that accounts the unequal role of geometric and energy parameters of A and B – cations in formation of compound properties.

We show that this descriptor allows a forecasting the composition of perovskites with a large value of ionic conductivity.

## Results and discussion

In **Fig. 1** a good correlation between σ and Δ (for k = 2) is demonstrated in a wide range of σ (logσ: –7 ÷ – 0.5). To compare the role of the energy and geometric parameters in descriptor we analyzed separately the correlations "σ - $\Delta_1$" and "σ - $\Delta_2$". It was found that these correlations in the same interval of σ are much worse in comparison with correlation "σ - Δ". Moreover, we obtained that a correlation "σ - $\Delta_2$" is better than a correlation "σ - $\Delta_1$". Hence, it follows that the influence of energy parameters of A and B cations on ionic conductivity of considered perovskites is stronger in comparison with geometry parameters.

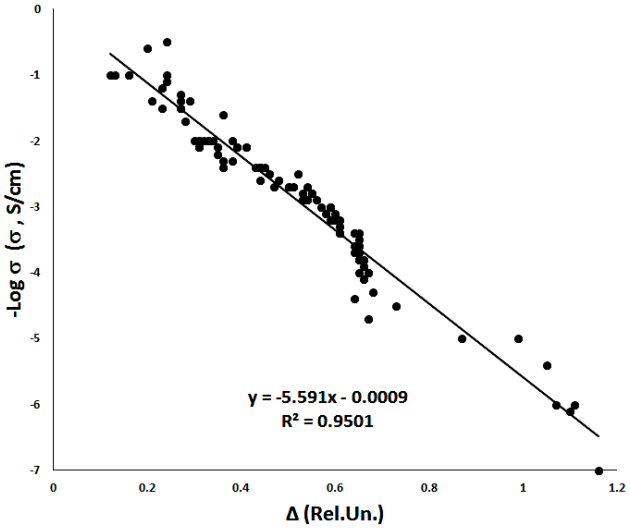


**Fig. 1.** Correlation dependence between log **σ** and Δ.

To get a better value for correlation coefficients in cases "log σ - $\Delta_1$" and "log σ- $\Delta_2$" we excluded a part of compounds from the list in **Table 1**. It turned out that we had to exclude more compounds in the case "log σ - $\Delta_1$" in comparison with the case "log σ - $\Delta_2$". As a result of this selection procedure the good correlation dependences shown in **Fig. 2** were obtained. The correlation graphs are intersected, and the intersection point corresponds to log σ = -0.82. It means that the best values of σ should be expected for compounds in the vicinity of the intersection point for two lines $\Delta_1$ and $\Delta_2$.

**Table 2**. Division of the list of compounds (Table 1) into the intervals of Δ.

| No | Δ | $R^2$ |
|---|---|---|
| 1 | 0.24 – 0.38 | 0.3352 |
| 2 | 0.38 – 0.50 | 0.6821 |
| 3 | 0.50 – 0.73 | 0.7887 |
| 4 | > 0.73 | 0. 8097 |

The list of compounds in **Table 1** was analyzed with respect to the ratio of correlation coefficients for different intervals of Δ. The correlation coefficients were calculated for intervals Δ shown in **Table 2**. One can see that for the region of larger magnitudes of σ the obtained correlations are worse. It follows that the correlation series should be selected based on the desired values of σ. For example in

 

the first interval of Δ (**Table 2**) to improve the correlation the number of compounds in the given interval Δ should be increased or some compounds should be excluded as shown in **Table 3**.

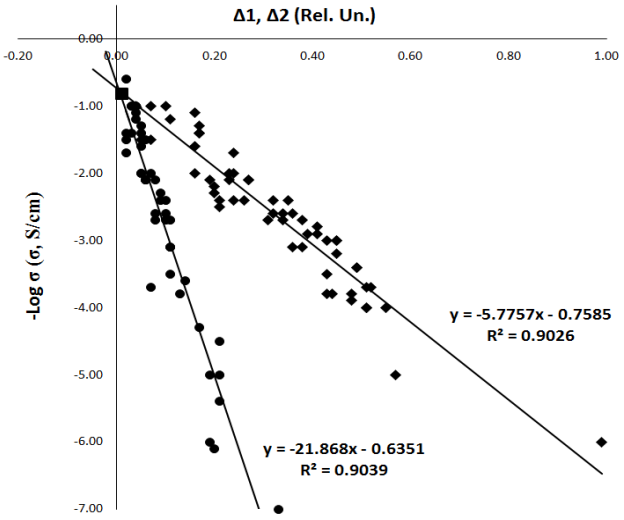


**Fig. 2.** Correlation dependences "log **σ** - $\Delta_1$" (circles) and "log **σ** - $\Delta_2$" (squares).

**Table 3**. Correlation selection of perovskites for interval 1 from Table 2.

| No | Removed compound | $R^2$ |
|---|---|---|
| 2 | $(La_{0.72}Nd_{0/08})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}$ $O_3$ | 0.3903 |
| 7 | $(La_{0.9}Nd_{0.1})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}$ $O_3$ | 0.7696 |
| 9 | $(La_{0.9}Cd_{0.1})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}$ $O_3$ | 0.9066 |
| 16 | $(La_{0.9}Yb_{0.1})_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}$ $O_3$ | 0.9476 |

In **Table 3**, as an example, we present a list of compounds that had to be excluded in order to increase the correlation coefficient in the first interval from **Table 2**. It can be seen that these compounds include the largest number of elements: two A – elements and three B – elements. We can assume that in these cases the averaging of parameters (RA, RB, VA, and VB) in the calculation of the descriptor is not quite correct.

## Conclusion

A descriptor which allows selecting perovskites with large values of ionic conductivity is constructed. This descriptor is a combination of radii and potentials of ionization of A and B cations in $ABO_3$ perovskites with only non-transition elements.

An approach of the correlation selection of perovskite compounds is proposed for the improvement of the correlation series and revealing compounds with deviating properties. Two ways to realize the proposed approach are demonstrated: lengthening the correlation series and exclusion of inappropriate compounds. The resulting correlation series allows determining a composition of perovskites with the desirable ionic conductivity.

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