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Big data approach for effective ionic radii ☆

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ABSTRACT

Effective ionic radii are a useful tool for researchers in many disciplines. These radii are usually determined from interatomic distances and the values tabulated by Shannon and Prewitt are widely used since 1969. Here, we present a modern approach based on automated queries to materials databases followed by categorization and tabulation. This method is used to augment the available set of effective ionic radii by providing radii for missing anionic oxidation states and coordination numbers. Our approach proves to yield results that are consistent with known values for anions with well-established oxidation states. More exotic cases result in larger uncertainties due to the smaller amount of available structural data. Nevertheless, the provided estimates give reasonable values for cases that are untabulated at present. Furthermore, our approach is designed to continuously improve together with the growth of available databases. Furthermore, small tweaks of the presented application will allow us to also complement or revise ionic radii of cations. Thus, our approach is designed to update the old and useful concept of effective ionic radii, bringing it to modern days.

Program summary

Program Title: `extend_anionic_radii.py`
Program Files doi: http://dx.doi.org/10.17632/sp4c25z8pn.1
Licensing provisions: LGPL-3.0
Programming language: `Python3`
Supplementary material: The database of ionic radii is available online, preliminary under https://extend-sp-radii-new.herokuapp.com.
Nature of problem: Determine the effective ionic radius for elements in anionic oxidation states (OS), depending on the coordination number (CN). This is done by harvesting the Materials Project (MP)[1] database. Newly found radii are adopted in a way that they coincide with reference values of the established Shannon–Prewitt (SP)[2] table for ionic radii.
Solution method: For an element X in oxidation state OS, find all binary compounds contained in the MP that are composed by X and alkali or alkaline-earth metals. Determine OS and CN for all elements in each of the identified binary compounds (assume OS=+1 and +2 for alkali and alkaline-earth metals, respectively). Determine the nearest neighbor distances between the elements. From the obtained information and the SP reference values, compute the effective ionic radius of X, depending on OS and CN.

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1. Introduction

Ionic radii are an effective tool for researchers in all fields related to materials science. The concept of describing solids as being constituted by ions (or atoms) with assigned electronic charge and, hence, the assignment of oxidation states is an approximate model. However, this concept proves to be very useful in many areas and

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it can be shown to be rigorous for band insulators. Consequently, since the beginning of the Twentieth century, great minds have dealt with this issue [1–7], leading to the seminal work of Shannon and Prewitt (SP) [8], who established a set of effective ionic radii for a large number of elements, oxidation states (OS), and coordination numbers (CN). While technically only constructed for oxides and fluorides, these radii are widely used today. Similar concepts have been used to establish effective radii for sulfides [9] and nitrides [10]. In addition to (inorganic) atomic ions, recently interest also grew to establish effective ionic radii for organic ions [11–13]. Despite its scale and successful widespread use, the SP set of radii is incomplete and does not cover all areas of the periodic system or desired combinations of OS and CN. Since the revised table of Shannon in 1976 [14], a large amount of additional data has been accumulated. Furthermore, in addition to growing experimental data, we now also have access to growing computational data with increasing level of accuracy. Density-functional theory (DFT) [15] is a powerful tool that is able to describe structural properties with sufficient accuracy for a wide range of materials. In recent years, great efforts were made to archive these data in databases [16–21]. Besides providing storage and transparency of computational results, these archives can also be used to harvest data in order to gain secondary insight. Such a big data approach is presented here in order to establish ionic radii for elements, OSs, or CNs that are missing in the SP table. To that end, we harvest the data contained in the Materials-Project (MP) [22] via the provided application programming interface (API), which currently contains almost 70,000 inorganic compounds. Here, we focus on establishing effective ionic radii for anions by accessing the available information for binary alkali and alkaline-earth metal compounds. To that end, we access a subset of 569 suitable crystals. Our `python` program then extracts the necessary geometric information and assigns CNs. By subtracting SP radii of the metals, we can determine and add unknown anionic radii into the established list of SP [23]. This approach is able to constantly evolve together with data archived in the MP. We demonstrate the linearity between ionic radius r_{ionic} and CN for halides and chalcogenides and complete the SP table for these elements. For completeness, we also apply our method for groups XIII (boron) to XVI (chalcogens) for all anionic OS up to a filled valence p shell. Furthermore, we provide estimates for transition metals in unusual anionic OSs. The resulting ionic radii are stored in a `postgresql` database, which will be made available for the public using a `django` based web application (see supporting information for details).

2. Results and discussion

An outline of our application is given in Fig. 1. Determination of a target ionic radius $r(\text{X})_{\text{OS,CN}}$ for an element X proceeds in the following steps:

1. Specify target elemental species X and OS.
2. Obtain all binary compounds M_mX_x, with M an alkali or alkaline-earth metal, from the MP.
3. Store the obtained structural data in form of the Crystallographic Information File (.cif) and process it in order to get the nearest-neighbor (NN) distances for X and M.
4. Use this information to determine $\text{CN}_i(\text{X})$ and $\text{CN}_i(\text{M})$ for every reference compound i.
5. From the obtained CN_i and the composition, determine $\text{OS}_i(\text{X})$, assuming $\text{OS(M)} = +1$ or $+2$ for alkali and alkaline-earth metals, respectively.
6. With $\text{OS}_i(\text{M})$ and $\text{CN}_i(\text{M})$ in hand, obtain the SP radius $r_i(\text{M})_{\text{OS,CN}}$. If not tabulated, obtain it from interpolation/extrapolation of the available SP radii.
7. Determine $r_i(\text{X})_{\text{OS,CN}}$.

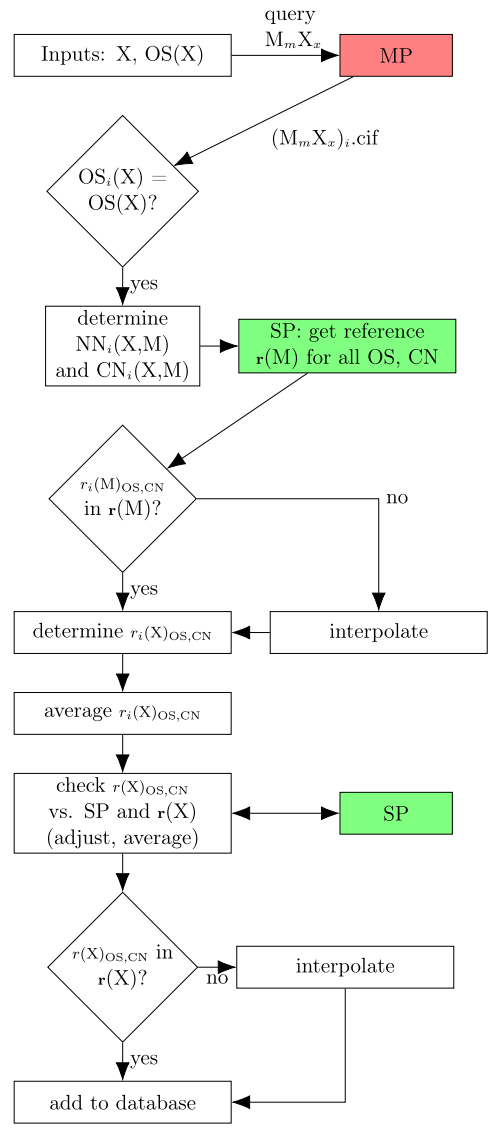

Fig. 1. Flow-chart of the presented application that uses the MP (red) and the SP table (green) as external sources. With these inputs, the ionic radius $r_{\text{ionic}}(X)_{\text{OS,CN}}$ of any given element X in an oxidation state OS is determined as a function of CN, depending on the availability of alkali and alkaline-earth metal reference compounds. The index i denotes the reference compounds, whereas the set of tabulated effective radii for all OS and CN for a given element is denoted by $\mathbf{r}$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

8. Collect the data for all compounds; multiple entries for any one OS and CN are averaged. If another CN(X) for the given OS(X) is contained in the SP set, adjust the data by a constant factor so that a fit containing old and new data retains the SP value. If $r_i(\text{X})_{\text{OS,CN}}$ does not increase with CN, average the data points.
9. Last, all $r_i(\text{X})_{\text{OS,CN}}$ are added to our database of SP radii. In addition, if CN = 6 or 12 are missing, these points are obtained by interpolation/extrapolation from the obtained data.

In its current form, our application is able to determine unknown effective anionic radii for use in conjunction with the SP table. We would like to emphasize that this choice has been made to comply with the very established SP reference, i.e., no value of SP is altered in the current table. Note that as a result, additional

influences like covalency (i.e., the bonding partner) [9,10,12] or temperature [24] are not contained in the present model. In the future, our approach may be used to revisit effective ionic radii for all cases and to include these effects. In addition to the approximations underlying the SP table, our basic assumption is that alkali and alkaline-earth metals are always found in OS $= +1$ and OS $= +2$, respectively. While this is justified for many cases, metallic bonds often display mixed covalent and ionic bonding character and, therefore, allow only the assignment of fractional OS (e.g., Laves phases [25]). Hence, in these cases the notion of ionic radii (at least based on integer OS) must be treated with caution and can only be seen as rough estimate. Furthermore, the influence of different reference metals is currently averaged. Similarly, cationic radii can be obtained by minor tweaks and the assumption that, e.g., halides are almost always found in OS $= -1$.

We start by determining missing CNs for halogen anions in OS $= -1$. While for F^- no action is needed, since the dependence of the ionic radius on CN was established by SP, only CN $= 6$ has been reported previously for the remaining halides. Our approach is able to provide the missing influence of CN for these cases. The agreement between SP and our value determined for CN $= 6$ is good, i.e., only small shifts of 0.04 Å (I^- and Br^-) and 0.02 Å (Cl^-) are needed to retain the SP values. On one hand, this confirms the accuracy of the established SP values; on the other hand, this validates our approach. The results for monovalent halides are summarized in Fig. 2 (a).

For most cases, our approach yields values that are determined with high accuracy and small error bars for CNs between 2 and 6. The resulting data can be fit linearly with good accuracy, allowing to extrapolate toward larger CNs. Furthermore, the slope of the linear fits is quite consistent for all halides, leading to a well-behaved averaged increase of the radii from CN $= 6$ to CN $= 12$ of $4.7 \pm 0.4\%$.

With these encouraging results, our procedure is applied to divalent chalcogenides (Fig. 2 (b)). Once again, for all cases but Te^{2-} the available data allows to determine relations between ionic radius and CN that behave linearly, with data points that show modest deviations from linearity. However, here the data points are concentrated on three CNs (4, 6, and 8). Due to the established linearity between CN and r_{ionic} for halides and the SP values for O^{2-}, the obtained linear behavior and the resulting values should still provide good estimates for r_{ionic}. Furthermore, the increase of r_{ionic} from CN $= 6$ to CN $= 12$ of $4.8 \pm 2.4\%$ is comparable to the halides, although the spread is increased significantly. Nevertheless, the overall increase of r_{ionic} from CN $= 6$ to CN $= 12$ combining data of halides and chalcogenides of $4.7 \pm 1.7\%$ (0.79% per CN) should be a reasonable approximation to the influence of CNs on r_{ionic}. In order to choose a lower bound that should be safe to not overestimate this influence for most cases, we choose an increase of $m = \frac{dr_{\text{ionic}}}{d\text{CN}} = 0.7\%$ for cases where not enough data points are present to allow an independent fit.

Next we investigate whether or not the relation between oxidation state and r_{ionic} also remains linear. While this was shown by SP [8] for different positive oxidation states, we are interested in generating radii for anionic oxidation states. In Fig. 2 (c) we compare the relation between OS and r_{ionic} for chalcogenides (note that we do not consider oxygen, since the latter is mainly found in OS $= -2$, and peroxo species are strongly covalent). Beyond the rough trend that anions have much larger ionic radii than cations, we find that the linearity becomes poor when combining cationic and anionic oxidation states. Therefore, the anionic oxidation states that are determined for metallic species below, cannot be reliably validated by any relation to the established cationic states. In addition, the ionic radii for chalcogenides width OS $= -2$ are slightly smaller than the ones obtained for OS $= -1$, which is counter intuitive. In part, this is a result of the shifting of OS $= -2$ values to the SP values. However, this shift is (as discussed) small for all chalcogenides and the obtained radii for OS $= -1$ remain slightly larger even after accounting for this shift. However, although chemical intuition would suggest an opposite trend, there

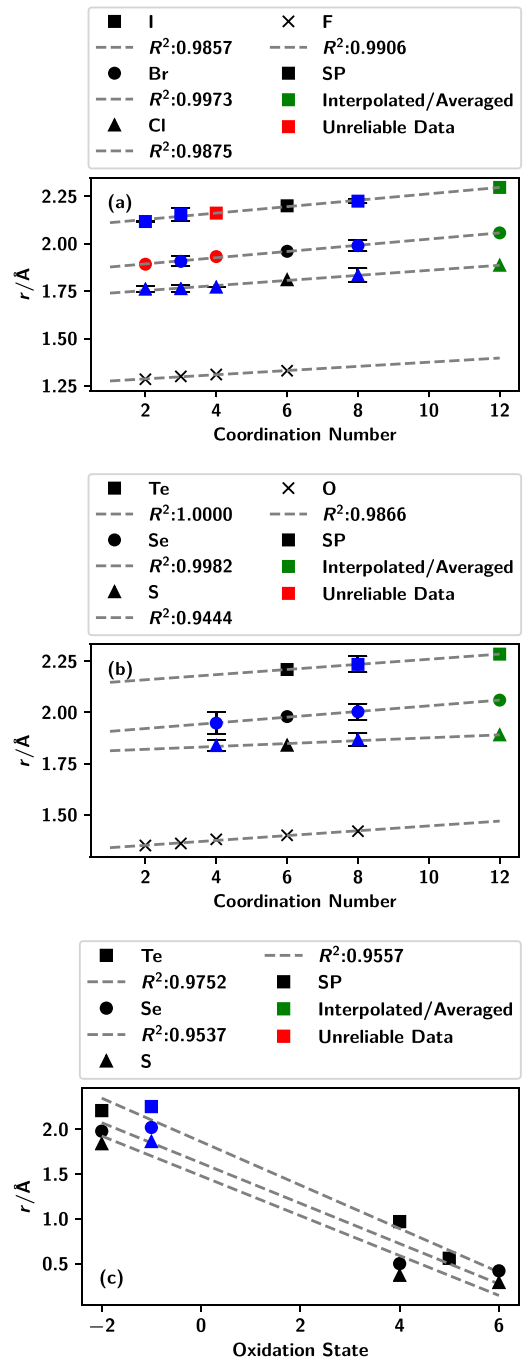

Fig. 2. Evaluation of r_{ionic} vs. CN for halides with OS $= -1$ (a) and chalcogenides with OS $= -2$ (b). Data points established by our method are in blue, with standard deviations determined for the set of available reference compounds in the MP. Whenever only one reference compound is found, the data point is marked unreliable (red). Values that result from interpolation or merging two neighboring data points (see text for details) are marked green. Data points from the original SP table are black. A linear fit for each data set is shown (gray) together with its correlation coefficient (note that $R^2 = 1$ results trivially for cases with too few data points). The dependence of r_{ionic} on OS is displayed for chalcogenides with CN $= 6$ in (c). The linear relation changes drastically when anionic OSs are considered together with cationic OSs. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

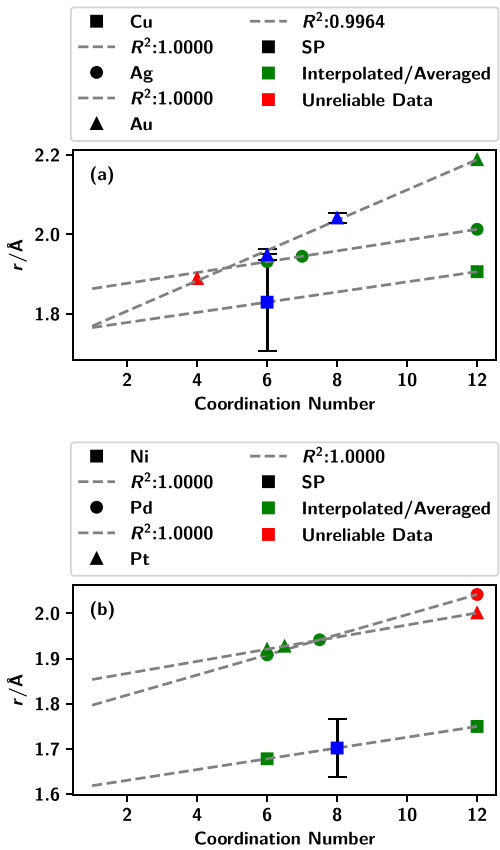

Fig. 3. Influence of CN on r_{ionic} for group XI^- (a) and X^{2-} (b) anions. While the available reference compounds allow for an evaluation of Au^- with good accuracy, the evaluation of other elements is limited by the small sample size of appropriate binary compounds.

is no example confirming this in the SP table. As only related trend one can compare the radii of O^{2-} and OH^-. A very small increase of 0.02 Å to 0.03 Å is observed in the higher OS. Such nuances are yet beyond the accuracy of our approach and possibly the original SP values. In addition to a refined approach that operates without the SP values as reference, such effects might be captured when taking into account the partner element in each binary compound, which has been shown to affect the effective ionic radii [12].

Nevertheless, our tests show that our approach gives sensible estimates for anionic radii for halides and chalcogenides that are in agreement with the SP values. Therefore, we can apply our approach also for elements where anionic radii have not been determined yet. Here, we show results for two groups of transition metals, namely for X^{2-} and XI^- anions. Note, however, that anionic radii for these cases have not been tabulated in previous attempts for a reason: On one hand, these OSs are, to some extent, exotic for these elements and are not found in as many materials as other OSs or anionic OSs in, e.g., halides or chalcogenides. Thus, the number of suitable crystal structures is naturally small, which reduces the accuracy of our method. On the other hand, most inorganic metallic bonds are a complex combination of ionic and covalent bond character. This leads to noninteger OSs and complicates the determination of the latter. Nevertheless, determining sizes of such "ions", as long as there is a significant ionic contribution to the bond, is often desired, and our present approach provides a first step towards this goal. As mentioned above, improvements could be made by including the bonding partner as additional variable to $r_i(X)$, taking into account electronegativity differences between elements, or by employing an automatic charge analysis to our method, once the required electron densities (or wave-functions) are added to existing archives, as it is possible, e.g., in NOMAD [18]. Here we discuss the present estimates, noting that cases where no error analysis could be performed should be treated with caution and only as rough estimates. The relations between CN and r_{ionic} are shown in Fig. 3. Fewer available compounds lead to a worse description for Cu^- and Ag^- compared to halides, and no relation between CN and r_{ionic} can be determined from the available data yet. Since at least CN = 6 could be determined for these cases, we apply the adjusted linear trend determined for halides and chalcogenides (see above) to extrapolate to other CNs. For Au^-, we obtain data points for CN = 4, 6, and 8; two of these are determined with good accuracy. The resulting relation with CN is again linear. The slope is much steeper (2.1% per CN) than the one obtained on average for halides and chalcogenides (0.79% per CN). This would suggest to alternatively apply the same slope to all members of a group if possible. For now, we keep our initial approach, relying on evolving the underlying database in the future.

A similar picture is also obtained for group X^{2-} ions. The limited data points again allow to reliably evaluate the target oxidation state only for one CN in the cases of Pt and Ni. Therefore, the other CNs are again obtained by the linear fit based on the results of halides and chalcogenides. As indicated by the results for Pd^{2-} (and Ag^- above), the true influence of CN might be underestimated for these cases.

For completeness, we also generated radii for elements in groups XIII (boron) to XVI (chalcogens) for OS −1 up to a filled valence p shell. As discussed for the previous examples, there are cases where the available data allows a good estimate, others where the data is very scarce or non-existing, leading to bad guesses or a failure of our approach. In some cases, the available data lead to a negative trend between CN and r_{ionic}. As noted above, this relation is much less pronounced for anions than for cations. Nevertheless, this indicates that further refinements and efforts to increase the underlying database are necessary for these cases. However, besides a lack of data, this is also perhaps due to these OSs being unstable, which obviously raises the question of whether determining these particular ionic radii is of significant value.

3. Details of the implementation

In this section we describe some of the steps outlined above in more detail for completeness.

3.1. Obtaining data

The raw data are obtained by accessing the MP using `pymatgen` in our `python` implementation. A query is performed for binary materials M_mX_x that contain the investigated element X and one additional element from the list of alkali and alkaline-earth metals. If the stoichiometry of the ith material does not fulfill the condition

$$\frac{m_i \mathrm{OS}_i(\mathrm{M})}{-\mathrm{OS}(\mathrm{X})} = x_i \,, \tag{1}$$

X is not in the OS we are looking for and, therefore, compound i is discarded.

3.2. Determination of CN

After obtaining the `.cif` files of target compounds with X in the correct OS, the geometry is processed. Nearest neighbor (NN) lists are obtained for each atom in the unit cell, excluding atoms of the same element. We take periodic boundary conditions into account by translating each neighboring ion into each adjacent unit cell. From this initial list, the minimal distance is obtained

for each case. Only this minimal distance and distances within a small threshold (0.3 Å) are considered in the next steps. The distances are averaged and their number is used to determine $CN_i(M)$ and $CN_i(X)$. If this procedure leads to inequivalent CNs for one of the elements, the respective compound is discarded. This happens, e.g., for cases of charge disproportion, which are less clear to interpret and unwanted at this stage. Furthermore, if the resulting averaged bond lengths differ by more than a threshold of 0.001 Å, the resulting CNs are checked for each case against chemical intuition.

3.3. Determine radii for unknown reference OS/CN

If a target $r(M)_{OS,CN}$ cannot be obtained (either because it is missing from the SP table or because no material is reported in the MP with the desired OS/CN combination), we use linear interpolation/extrapolation from the available data. Thus, for a species S we simply solve

$$r(S)_{OS,CN} = m\mathrm{CN}(S) + t \,, \tag{2}$$

where $m = \frac{dr(S)_{OS,CN}}{d\mathrm{CN}(S)}$ and t are determined from the available data to a given OS. Linear interpolation is usually a very good approximation within a moderate range of CNs. For now, we implemented the following adjustments to Eq. (2): If OS exists in the SP table, t is adjusted in a way that the new value coincides with the old SP value. This shift is then also applied for all other CNs. Furthermore, if the radius to a given CN is larger than the radius of the next higher CN, then these data are not trusted. Radii and CN of the respective pair of CNs are averaged and the individual data are discarded, unless one of the two data points is from the SP table. In that case, the SP value is chosen, and the other one discarded. These tweaks ensure that new radii are fully compatible with the established data set of SP. A revision of this process and the whole set of ionic radii should be possible in the future.

In cases where interpolation is not possible because only one data point is available, we scale the radius with respect to CN. As explained above, the data of halogens and chalcogens would suggest an increase by 0.79%, i.e., a scaling factor of $m = 0.0079$. Albeit this is not perfect, a scaling with respect to this average should allow to give a reasonable estimate for the influence of CN on r_{ionic} for most cases. In order to not over estimate this approximative effect, we chose a smaller scaling factor of $m = 0.007$. As seen by the deviations in the available data for Au^- and Pd^{2-}, this cautious choice indeed seems to underestimate this effect for group X and XI elements. With increasing data or by including cationic oxidation states, we hope to establish better relationships per element or periodic group.

4. Conclusion

We present a modern implementation using data harvesting to continue the work of SP in order to estimate ionic radii. We focus on anionic radii, completing the relationship between CN and r_{ionic} for halides and chalcogenides. Furthermore, novel anionic radii for transition and main group metal elements are obtained. Although the accuracy of the latter is yet limited, due to the smaller sample size for these elements in anionic oxidation states compared to halides and chalcogenides, our approach allows a continuous improvement of the estimated ionic radii with the growth of the chosen database (MP) or an extension to other databases. Furthermore, the outlined approach should allow sensible estimates for researchers in need of ionic radii for these kinds of exotic ions and oxidation states. For example, the estimated ionic radii provided good guidance in our quest of designing inverse-hybrid perovskites [26–28].

Despite the success of SP radii and this application aimed to complete this set of radii, the benefit of additional data and evolving data methods should also enable to improve on the values of the SP table. Our application can be used to do so, since it can also be used to determine radii for cations by small adjustments. By intensive analysis of the data, deviations from regular trends and errors, we plan to revise the full table of ionic radii in future work. Further dependencies of r_{ionic} on the bound element [12] or temperature are possible [24]. Additional charge analysis could further improve the results and add a measure for covalency to the ionic radii. The resulting database of ionic radii is available online (see supporting information).

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Conflicts of interest

There are no conflicts to declare.

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