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Universality in size-driven evolution towards bulk polarizability of metals†

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Abstract. The properties and characteristics of materials on the subnano/nano scale are very different from those of their bulk counterparts. The evolution of materials properties with size is the holy grail of nanoscience. An intriguing question then is: Can one predict what type of material (metal, semiconductor or insulator) an unidentified element will be, when in bulk quantities, solely from the properties it exhibits over a limited range of the subnano/nano size-regime? We demonstrate here that for nominally metallic elements (i.e., elements that are metals in bulk quantities) the answer to this question is "yes", and the very identity of the element also can be established. Most importantly, we show that the phenomenon of size-induced transition to metallicity, as gauged by polarizability, is characterized by features and trends that are universal for all metals. Combining numerical simulation data with an analytical model we introduce a universal constant and derive equations that express the universality explicitly.

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The type of a bulk material - metal, semiconductor or insulator - can be identified using various physical properties (electronic, magnetic, optical), or, alternatively, the way a material responds to an external perturbation, for example, an external electric field. From the electronic point of view, metals are materials with zero gap between the valence and conduction bands; in non-metals this gap has a non-zero value. In terms of response properties, metals are materials in which an external electric field leads to separation of charges, so that the net effect is expulsion of the field from the interior of a metal (the Faraday cage effect). In non-metals, the field induces polarization of charges that results in reduction of the field in the interior of a non-metal, but not complete screening.

Identification of types of materials on the nanoscale is not as straightforward. In fact, even though the term "nanomaterials" is broadly used in nanoscience and nanotechnology, the discipline of *nanoscale materials science* is yet to be developed. One of the reasons for this state of affairs is that elements and compounds when in "nanoquantities" behave very differently from their bulk counterparts. For example, small and medium size atomic clusters of nominally metallic elements (i.e., elements that are metals in bulk quantities) as a rule lack altogether the properties characteristic of metals. These properties then grow in as the clusters grow in size. The phenomenon is known as the size-induced transition to metallicity (see, e.g., Refs. 1-4 and citations therein).

The size at which a cluster of a metallic element becomes a metal depends on the property/descriptor used to gauge the transition. A cluster may behave as a metal as judged by one descriptor and as a nonmetal as judged by another. The *bona fide* metallic state is attained at a size, or size-range, at which all the properties become those of the corresponding bulk metal. The property used most extensively in the previous studies, both experimental and theoretical, is the finite-size analog of the bulk bandgap (see, e.g., Refs. 3-4 and citations therein).

In neutral clusters, this analog is the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). In anionic clusters - systems that are actually interrogated in experiments (the dominant technique is that of electron photodetachment; see, e.g., Ref. 4 and citations therein), it is the gap between the energies (or, equivalently, binding energies) of the two most external electrons.[3,5] In the small and medium size regime, these two gaps are not necessarily the same, or even close, because the preferred structure of an anionic cluster may be different from that of its neutral counterpart. The two gaps, however, converge to each other and to the bulk bandgap as the clusters increase in size.

The details of and the trends in the evolution towards bulk material properties as a function of system size depend on the elemental composition. One can then pose an intriguing fundamental question: Can features and trends in the size-evolution of properties over the range of small and medium sizes, where the properties are still very different from those of the corresponding bulk limit, be used to identify/predict what type of material a system will become as it grows from the nanoscale to the bulk regime?

In this Communication, using density functional theory (DFT) based calculations and model considerations, we demonstrate that the answer to this question is "yes" for elements that are metals in bulk quantities. Specifically, we show that small and medium size clusters of these elements, when analyzed in terms of their polarizability (more precisely, the so-called local, or dipole, and charge-transfer components of polarizability[6]), exhibit general size-dependent trends that have universal validity as identifiers/predictors of the metallic nature of these elements in the bulk limit. We introduce a constant that is universal for all metallic elements and derive equations that predict that the bulk metallic state is attained, as gauged by polarizability, as the size of the systems increases, with the same universal rate for all metallic elements.

The polarizability data were generated for clusters of Na, K, Al, and Zn as representatives of alkali (Na and K), s-p (Al), and transition (Zn) metals. The computational details together with a brief recap of the scheme for atomic-level analysis of polarizability[6] are given in the Electronic Supplementary Information. The scheme also provides for partitioning the total polarizability of a finite system into the so-called local, or dipole, and charge-transfer components,

$$\alpha_{ij} = \alpha_{ij}^{p} + \alpha_{ij}^{q}, \tag{1}$$

where α_{ij}, α_{ij}^{p} and α_{ij}^{q} (i, j = 1, 2, 3 or x, y, z) denote elements of the total polarizability matrix and its dipole and charge-transfer parts, respectively. The dipole components α_{ij}^{p} characterize a dielectric type of response of a system to a vanishingly small external electric field, whereas the charge-transfer components α_{ij}^{q} serve as a gauge of a metallic type of response. The analysis presented below is performed in terms of the directionally averaged (rotationally invariant) polarizability $\langle\alpha\rangle = \frac{1}{3}\sum_{ii=1}^{3}\alpha_{ii}$ and its dipole $\langle\alpha^{p}\rangle$ and charge-transfer $\langle\alpha^{q}\rangle$ components, where α_{ii} are the diagonal elements of the polarizability matrix. For each element and cluster size - with the exception of the case of n=146 atoms (the largest cluster size considered) - we used the corresponding most stable geometric form (the details on the structural forms and their coordinates are given in the Electronic Supplementary Information).

As mentioned, our focus is on the issue of identification/prediction of the type of a macroscopic material solely from the properties of its subnano- and nano-scale precursors. Below we present results and an analysis that demonstrate that the conventional bulk metallic identity of elements can be predicted from the features exhibited by the static polarizability of their small clusters containing fewer than 100 atoms. More specifically, it is the particular trends in the size-evolution of the dipole and the charge-transfer components of the polarizability over this small size regime that have a universal validity as identifiers/predictors of a "future" (bulk) metal.

Figure 1 displays, as representative cases, the lowest energy structures of Na_n, K_n, Al_n, and Zn_n for n=20, 40 and 70, and that for n=146. As is clear from the figures, the preferred packing of atoms is both element and size dependent.

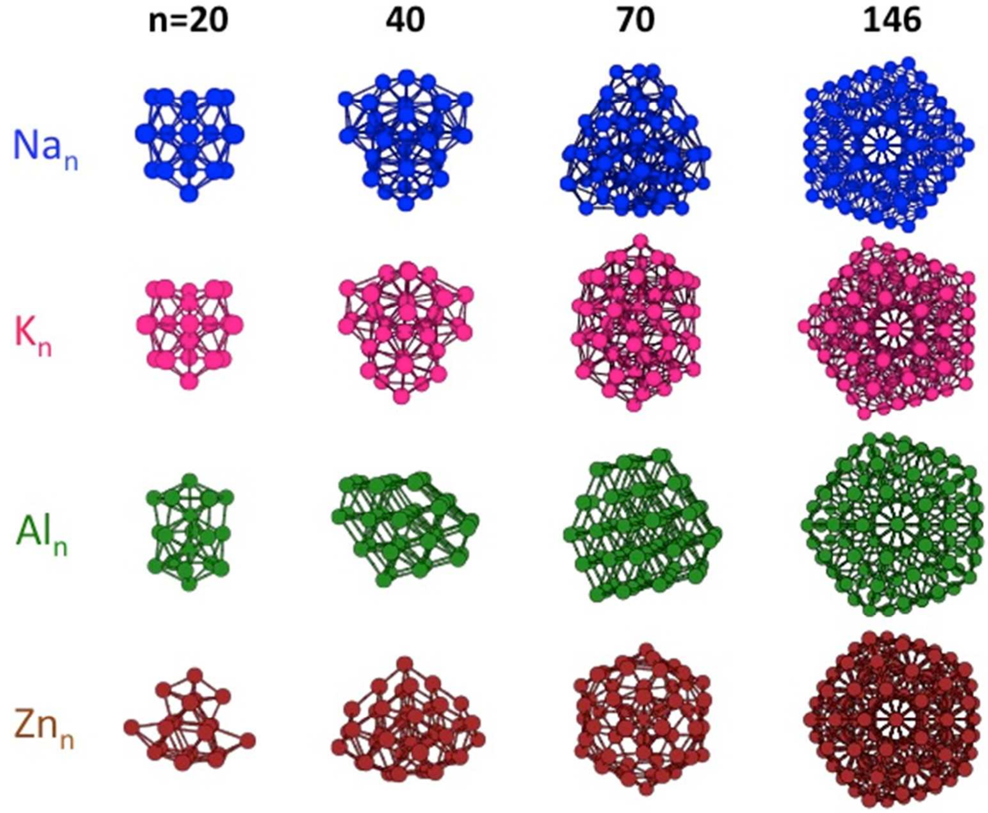

Fig. 1. Most stable structures of Na$_n$, K$_n$, Al$_n$ and Zn$_n$, n = 20, 40 and 70. The structures for n=146 are derived from the corresponding icosahedral 147-mers. See the Electronic Supplementary Information for details.

Figure 2 shows the graphs of the total polarizability per atom of Na, K, Al, and Zn clusters, as well as their dipole and charge-transfer components, as a function of cluster size. Several common features are apparent: 1) The total polarizability decreases, albeit non-monotonically, as the clusters grow in size; 2) the local departures from monotonicity originate entirely from the charge-transfer component; 3) the dipole component of the total polarizability is largely a smooth monotonically decreasing function of size; 4) the charge-transfer component shows a rapid initial increase followed by a "saturation" leveling off with an increase of cluster size; 5) the "saturation" value of the charge-transfer component agrees with the value of the bulk polarizability of the corresponding metal. Whereas these observations have been made for Na in our earlier study,[7] here we assert that they are general and valid for all metals.

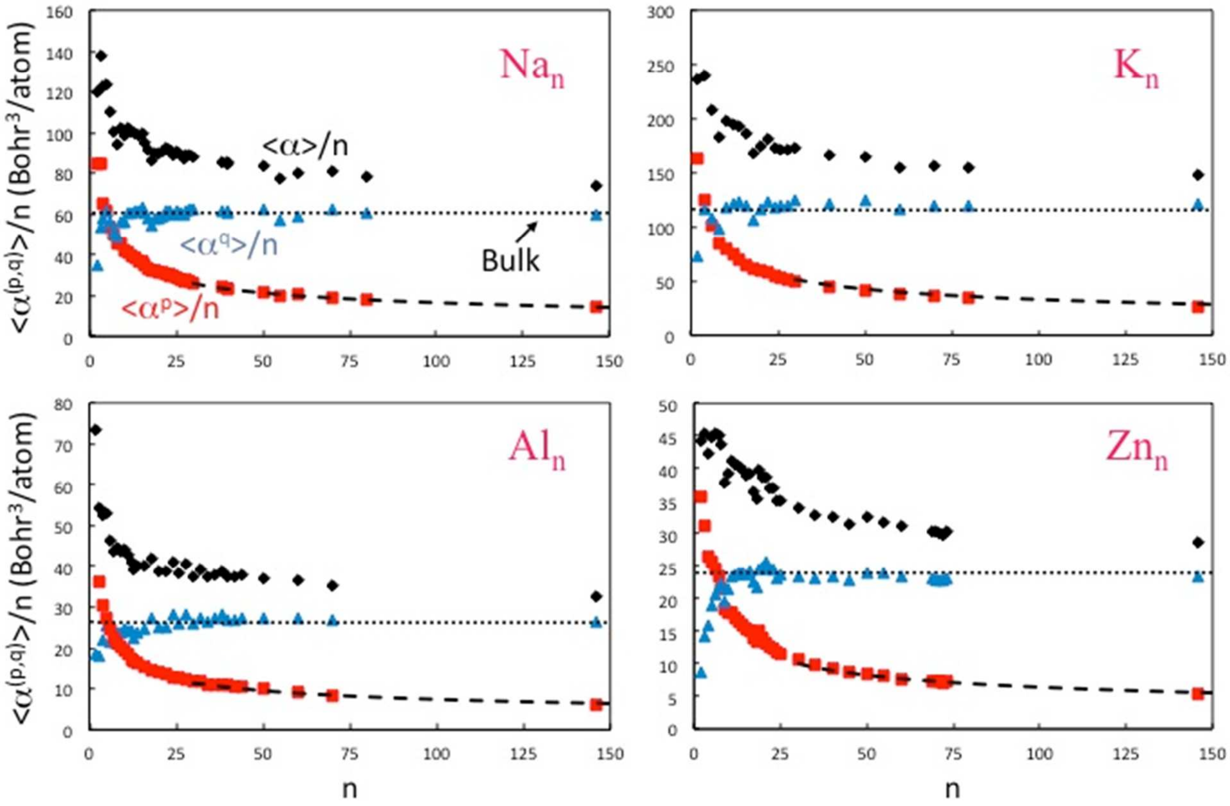

Fig. 2. DFT-calculated total $\langle\alpha\rangle/n$, charge-transfer $\langle\alpha^q\rangle/n$ and dipole $\langle\alpha^p\rangle/n$ polarizability per atom as a function of cluster size for Na$_n$, K$_n$, Al$_n$ and Zn$_n$. The dashed lines are graphs of Eq. (6'') with α_0 listed in Table 1 and ζ=0.39. The dotted lines represent the values of $\tilde{\alpha}_0$ listed in Table 1. See the text for details.

The most remarkable of the above findings is that, on a per atom basis, the charge-transfer components of the cluster total polarizabilities converge rapidly to the polarizability of the corresponding bulk metals. This happens when the systems are only about 20-25 atoms in size, which means that clusters of nominally metallic elements carry their element-specific true (bulk) metallic identity, as gauged by the charge-transfer component of their total polarizability, from very small, "embryonic" sizes. The quantity that makes their states, as defined by their total polarizabilities, different from those of the corresponding bulk metals is the non-zero contribution of the dipole components. With an increase of cluster size, the magnitudes of the dipole components decrease and eventually vanish, and the systems (elements) attain/reveal their bulk metallic identity.

The approach to full metallicity, as gauged by polarizability, can be quantified in terms of a measure we refer to as the *degree of metallicity* d_m defined as

$$d_m = \frac{\langle \alpha^q \rangle}{\langle \alpha \rangle} = 1 - \frac{\langle \alpha^p \rangle}{\langle \alpha \rangle}. \tag{2}$$

Since the approach is smooth, one needs to specify a threshold value. A cluster is considered to be fully metallic when the value of its d_m attains the chosen threshold, say 0.99 ($d_m = 1$ corresponds to the bulk metallic state). Figure 3 displays the graphs of the calculated d_m as a function of size for clusters of Na, K, Al and Zn. Even for n=146 the values of d_m are still quite far from 1. But the striking feature of the d_m graphs is that, except for the very small sizes, they essentially fall on top of each other for all four elements. This implies that all four attain the fully developed metallic state, as gauged by d_m, at the same size or, more robustly, size range.

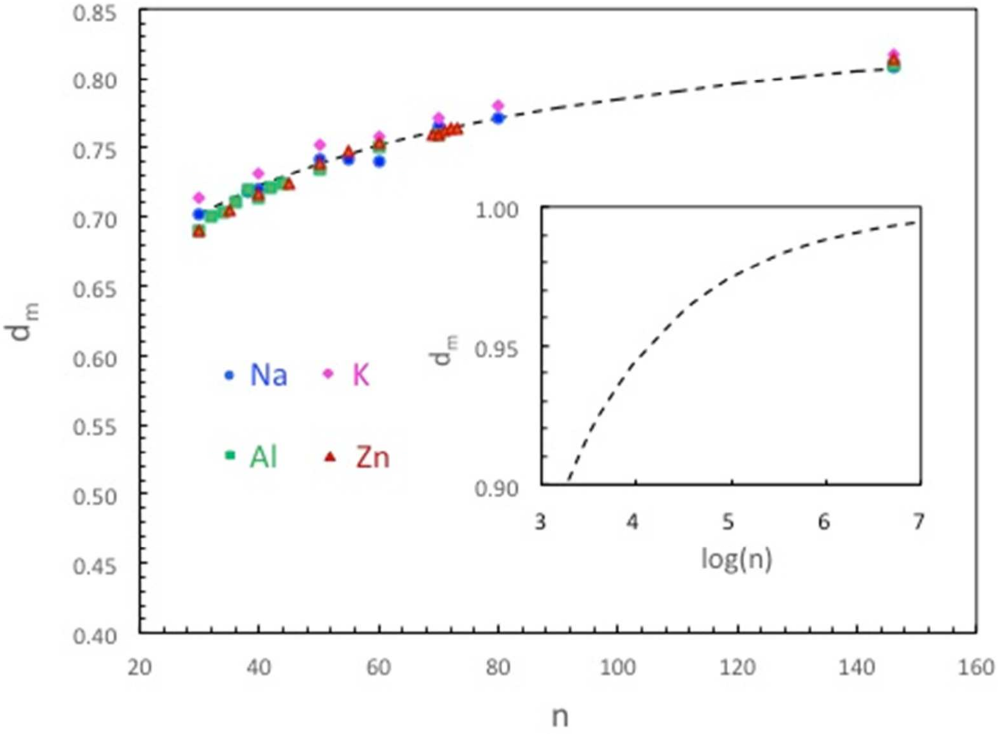

Fig. 3. DFT-calculated degree of metallicity d_m as a function of cluster size for $\mathrm{Na_n}$, $\mathrm{K_n}$, $\mathrm{Al_n}$ and $\mathrm{Zn_n}$**.** The dashed line is the graph of Eq. (8) with ζ=0.39. The inset shows the graph of Eq. (9) with ζ=0.39. See the text for details.

The above findings can be combined with and gain insight from the following model considerations. The total polarizability $\langle\alpha\rangle$ of a metallic sphere can be represented as (see, e.g., Ref. 8 and citations therein)

$$\langle\alpha\rangle=(R+\delta)^3, \qquad (3)$$

where R is the radius of the sphere and δ is the spillover parameter, which quantifies the spatial extension of the electronic charge density beyond the boundary of the sphere. On a per atom basis, the rhs of Eq. (3) can be rewritten as

$$\left(R+\delta\right)^3/n = R^3/n + 3R^2\delta/n + 3R\delta^2/n + \delta^3/n. \tag{4}$$

If the sphere is sufficiently large ($R \gg \delta$), δ in Eq. (3) can be neglected and, consequently, the first term in the rhs of Eq. (4) $R^3/n = \langle\alpha\rangle_{R\gg\delta}/n = \alpha_0$, where we identified $\langle\alpha\rangle_{R\gg\delta}/n$ as the bulk polarizability (per atom) α_0 of the metal. For clusters - except those of the smallest sizes – this translates into $R^3/n = \langle\alpha^q\rangle/n$ (cf. the discussion above). As a consequence, one identifies the last three terms in the rhs of Eq. (4) as representing $\langle\alpha^p\rangle/n$,

$$\langle\alpha^p\rangle/n = 3R^2\delta/n + 3R\delta^2/n + \delta^3/n. \tag{5}$$

With the substitution $R = \sqrt[3]{\alpha_0 n}$, Eq. (5) takes the form

$$\langle\alpha^p\rangle/n = 3\alpha_0^{2/3}\delta n^{-1/3} + 3\alpha_0^{1/3}\delta^2 n^{-2/3} + \delta^3 n^{-1} \tag{6'}$$

or, alternatively,

$$\langle\alpha^p\rangle/n = \alpha_0\left(3\zeta n^{-1/3} + 3\zeta^2 n^{-2/3} + \zeta^3 n^{-1}\right), \tag{6''}$$

where $\zeta \equiv \delta\alpha_0^{-1/3}$. In terms of ζ, the total polarizability per atom of an *n*-atom cluster of a metallic element can be written, except for the smallest sizes, as

$$\langle\alpha\rangle/n = \alpha_0\left(1 + 3\zeta n^{-1/3} + 3\zeta^2 n^{-2/3} + \zeta^3 n^{-1}\right). \tag{7}$$

Substitution of Eqs. (6'') and (7) into Eq. (2) leads to the following expression for the degree of metallicity d_m:

$$d_m = \frac{1}{1+3\zeta n^{-1/3}+3\zeta^2 n^{-2/3}+\zeta^3 n^{-1}}, \tag{8}$$

or in the limit of large *n*,

$$d_m \approx 1-3\zeta n^{-1/3}. \tag{9}$$

By fitting Eq. (8) to the DFT-calculated values of d_m one can obtain the value of ζ. The lower bound of the fitting domain is defined as the size at which $\langle \alpha^q \rangle / n$ reaches its saturation value and levels off (cf. Fig. 2). Over this domain, not only $\langle \alpha^p \rangle / n$ but also $\langle \alpha^q \rangle / n$ exhibits smooth scaling behavior.

A tacit assumption in the preceding considerations is that δ and, consequently, ζ do not depend on the system size, and therefore the fitting can, in principle, be performed at any size *n* from the scaling range. As an a posteriori justification for the assumption of size-independence of ζ one can use the fact that the calculated values of d_m and $\langle \alpha^p \rangle / n$ can be reproduced by, respectively, Eqs. (8) and (6'') with a constant ζ for all sizes in the scaling range very accurately (see below).

To avoid biasing the fitting by the possible residual effect of structure at small sizes and the inherent limitation on the accuracy of the calculated results specific to a single chosen size, the actual fitting of Eq. (8) was performed for each of the four elements considered here using the least-square procedure applied to the corresponding DFT-calculated data on d_m over the size range $n \geq 30$. The resulting values of ζ for Na, K, Al and Zn are listed in Table 1. A remarkable point to notice is that, notwithstanding the differences in the types of these metallic elements, their ζ values are essentially the same. We conjecture that ζ=0.39 – obtained as the average of the calculated values - is a universal constant common to all metallic elements. It establishes a universal proportionality relationship between the spillover parameter δ and the cube-root of bulk polarizability α_0 that holds for all metals. Since it is derived from numerical simulations, the value 0.39 should be viewed at this stage as a close estimate of the actual magnitude of ζ. A more accurate value may be expected to emerge from future analytical work.

The universality of ζ makes Eqs. (6''), (7) and (8) also universal. Equations (7) and (6'') state that the total polarizability per atom and its dipole component can be calculated for a cluster of any metallic element straightforwardly from the corresponding bulk polarizability of the element α_0 and size-dependent scaling factors $1+3\zeta n^{-1/3}+3\zeta^2 n^{-2/3}+\zeta^3 n^{-1}$ and $3\zeta n^{-1/3}+3\zeta^2 n^{-2/3}+\zeta^3 n^{-1}$ that are common for all metals. They also imply that the ratio of the total polarizabilities and that of the dipole components of the total polarizabilities for same-size clusters of any two metallic elements are size-independent and equal to the ratio of the corresponding bulk polarizabilities. Equation (8) makes it clear that the reason behind what appeared at first glance to be a striking coincidence of the d_m graphs in Fig. 3 is the universality (i.e., common value) of ζ. As is shown in Fig. 3, the calculated values of d_m are reproduced by Eq. (8) with ζ=0.39 accurately for all four elements and at all sizes within the scaling range; the individual point-wise discrepancies are within 1.7%.

With the value of ζ established, one can obtain the value of α_0 by substituting the calculated values of $\langle\alpha^p\rangle/n$ into Eq. (6'') or, alternatively, those of $\langle\alpha\rangle/n$ into Eq. (7). In principle, one can use the $\langle\alpha^p\rangle/n$, or $\langle\alpha\rangle/n$, value for any single size in the scaling range. However, because of the reasons mentioned above, we used the least-square fitting procedure applied to data sets in the size range $n \geq 30$. The values of α_0 for Na, K, Al and Zn obtained by fitting Eq. (6'') are listed in Table 1. The table also shows the values of $\overline{\langle\alpha^q\rangle/n}$ obtained by averaging the calculated $\langle\alpha^q\rangle/n$ data over the size range $n \geq 30$, as well as those of the bulk polarizabilitiy per atom $\tilde{\alpha}_0$ evaluated as $\tilde{\alpha}_0 = (3/4\pi)V_0$,[9] where V_0 is the bulk volume per atom, and the spillover parameter δ calculated as $\delta = \zeta\alpha_0^{1/3}$. Since the values of α_0 and $\overline{\langle\alpha^q\rangle/n}$ are obtained for equilibrated structures, they correspond to zero temperature. The values of $\tilde{\alpha}_0$ were calculated employing atomic volumes V_0 that were obtained using experimental low-temperature data on the bulk densities of Na,[10] K,[10] Al,[11] and Zn[12] and the atomic weights of the elements.

Inspection of the table reveals an excellent agreement between the α_0 and $\overline{\langle\alpha^q\rangle/n}$ values corroborating the identification of the saturation magnitude of $\langle\alpha^q\rangle/n$ as the bulk polarizability α_0. The calculated values of α_0 are also in good agreement with the experimentally based values $\tilde{\alpha}_0$ of the bulk polarizability for all four elements.

In addition to the DFT-derived data, Fig. 2 also displays the graphs of Eq. (6'') calculated with ζ=0.39 and the α_0 values listed in Table 1. The graphs reproduce the DFT values of $\langle\alpha^p\rangle/n$ for all four elements and all sizes within the scaling range well (the average point-wise discrepancies are 2.1% for Na, 5.7% for K, 2.8% for Al, and 2.0% for Zn; the larger discrepancy for K is a purely numerical effect the origin of which is in that its d_m values are slightly but systematically shifted from those of the other three elements, cf. Fig. 3, and the effective value ζ=0.39 is dominated by the latter – cf. also Table 1).

The inset in Fig. 3 shows the graph of Eq. (9) for large values of n. Using this graph and choosing d_m=0.99 as the threshold criterion, we estimate that the size at which clusters of metallic elements become fully developed metals, as gauged by their polarizabilities, is ~$1.57 \cdot 10^6$ atoms; for the threshold value d_m=0.95, this size reduces to ~$1.35 \cdot 10^4$ atoms. Should it turn out that for some metal, or metals (they may be called "exotic", if found), the value of ζ obtained as described above is different from the universal value 0.39, Eqs. (6''), (7) and (8) still remain valid for them, but should be used with the actual value of ζ.

The size, or size range, at which finite systems of metallic elements become fully developed metals, as gauged by polarizability, is significantly larger than that at which their HOMO-LUMO gaps close (and remain closed), as gauged, for example, by the energy gap of the order of kT (k – Boltzmann constant, T – temperature), - typically in the range of hundreds of atoms;[4] see the Electronic Supplementary Information for the size-evolution of the HOMO-LUMO gap of systems considered here. The dependence of the "critical" size, or size range, on the descriptor used to analyze the transition to bulk attributes is well appreciated. It is important, however, to also appreciate the subtle differences in the implications and meaning of the different descriptors. The HOMO-LUMO gap is viewed as a finite-size analog of the bulk bandgap. The zero bandgap in metals translates into their electrical conductivity. The closure of the HOMO-LUMO gap, however, does not necessarily mean that the finite system became a conductor, at least not in the sense of the traditional ballistic conductivity of metals. On the other hand, the transition to metallicity as analyzed above in terms of polarizabilty does define the size at which finite systems of metallic elements become metals in the sense that their polarizability approaches the polarizability of the corresponding bulk metal to a predefined degree.

As a final comment, we remark that the aspect of structure/shape plays essentially no role in the above considerations. The reason is that for clusters of metallic elements in the scaling range, the charge-transfer component $\left\langle \alpha^q \right\rangle / n = \alpha_0$ for all isomeric forms (even if the lower bound of the scaling range may be slightly different for different isomers), and the size-evolution of the dipole component $\left\langle \alpha^p \right\rangle / n$ towards zero is structure-insensitive (more details on this will be given elsewhere).

In summary, clusters of metallic elements already at remarkably small sizes of just a few tens of atoms display trends in the size-dependence of their polarizabilities that are universal. These trends are: a) size-independence of $\left\langle \alpha^q \right\rangle / n$: $\left\langle \alpha^q \right\rangle / n = \alpha_0$, where α_0 is the bulk polarizability of the metal; b) the size-dependences of $\left\langle \alpha^p \right\rangle / n$ and $\left\langle \alpha \right\rangle / n$ are fully defined by the bulk polarizability α_0 and the universal size-scaling factors that incorporate the universal constant ζ=0.39 as specified by Eqs. (6'') and (7), respectively; and c) a common for all metallic elements degree of metallicity d_m as a function of size, Eqs. (8) and (9), and consequently a common size at which they all acquire the bulk metallic state as gauged by a chosen threshold value of d_m. These trends can serve as criteria for identification of an unidentified element as a particular metal using solely the values of $\langle\alpha\rangle/n$, $\langle\alpha^q\rangle/n$ and $\langle\alpha^p\rangle/n$ calculated for its small clusters.

How many and which of these trends does one need to examine to arrive at a definitive identification? Examination of the dipole component $\langle\alpha^p\rangle/n$ alone may not be sufficient. As an illustration, we invoke the case of small to medium size Si clusters whose $\langle\alpha^p\rangle/n$ over the size range of n ≤ 147[13] mimics the discussed above trend to vanish exhibited by clusters of metallic elements. Si, however, is not a metallic element. Its DFT-calculated $\langle\alpha^q\rangle/n$ values in the size range 30 ≤ n ≤ 147 do not exhibit a trend of constancy – instead, they increase essentially monotonically with size – and, consequently, Eqs. (6''), (7) and (8) are not valid for it. The reason for the mentioned "misleading" behavior of the $\langle\alpha^p\rangle/n$ values is that for Si clusters the size range n ≤ 147 is still below the *asymptotic* scaling range that characterizes the approach to bulk Si (cf. Ref. 13). Can constancy of the charge-transfer component as a function of size be a sufficient condition for identification of an element as a metal? We lean towards the answer "yes", but it will need to be verified by future studies.

Conflict of interest

There are no conflicts to declare.

Acknowledgments

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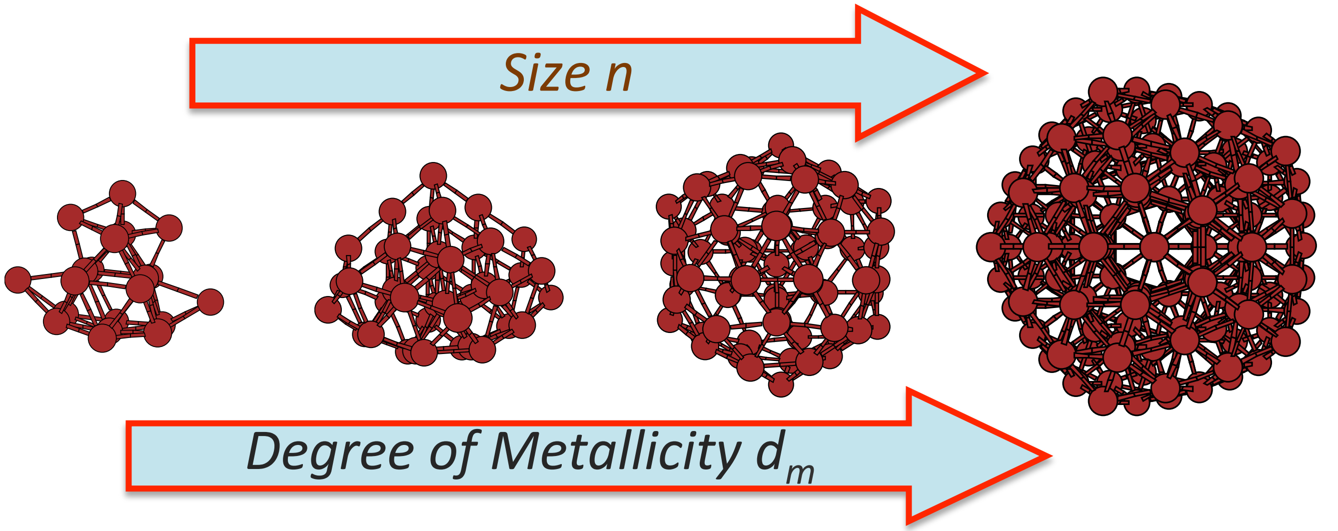
Table 1. The value of ζ obtained by fitting Eq. (8), bulk polarizability α_0 obtained by fitting Eq. (6'') with the listed ζ values, average DFT-calculated charge-transfer component per atom $\overline{\langle \alpha^q \rangle / n}$, bulk polarizability $\tilde{\alpha}_0$ obtained from measured bulk density and atomic weight of the element, and spillover parameter δ calculated from the values of ζ and α_0 (see the text for details). The polarizabilities are in units of Bohr^3 and the spillover parameter in Bohr.

Element	ζ	α_0	$\overline{\langle \alpha^q \rangle / n}$	$\tilde{\alpha}_0$	δ
Na	0.393	60.88	60.68	60.67	1.55
K	0.372	121.80	121.35	115.83	1.84
Al	0.399	27.05	27.00	26.26	1.20
Zn	0.395	23.40	23.30	24.00	1.13



Size n

Degree of Metallicity d_m

$$d_m = \frac{1}{1 + 3\zeta n^{-1/3} + 3\zeta^2 n^{-2/3} + \zeta^3 n^{-1}} \,, \quad \zeta = 0.39$$

The size-induced transition to metallicity, as gauged by polarizability-based descriptors, exhibits universal features.