Letter

Fine-Structure Constant Connects Electronic Polarizability and Geometric van-der-Waals Radius of Atoms

Alexandre Tkatchenko,* Dmitry V. Fedorov, and Matteo Gori

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ABSTRACT: The fine-structure constant (FSC) measures the coupling strength between photons and charged particles and is more strongly associated with quantum electrodynamics than with atomic and molecular physics. Here we present an elementary derivation that accurately predicts the electronic polarizability of atoms $\mathcal{A}$ from their geometric van-der-Waals (vdW) radius R_{vdW} and the FSC α through the compact formula $\mathcal{A} = (4\pi\varepsilon_0/a_0^{4}) \times \alpha^{4/3}R_{vdW}^{7}$, where ε_0 is the permittivity of free space and a_0 is the Bohr radius. The validity of this formula is empirically confirmed by estimating the value of α from nonrelativistic quantum calculations of atomic polarizabilities and atomic vdW radii obtained from both theory and experiment. Our heuristic derivation based on empirical data extends the influence of FSC from quantum electrodynamics and specific materials properties such as the visual transparency of graphene to atomic electronic properties throughout the periodic table of elements.
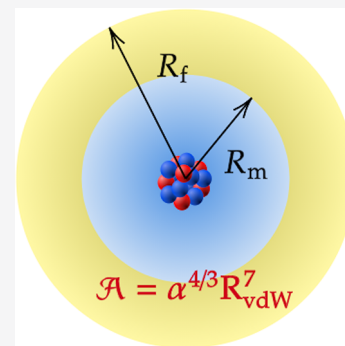
The fine-structure constant (FSC) is a dimensionless constant of nature that is thought to have remained spatially and temporally homogeneous throughout the evolution of the universe.[1,2] The FSC relates the properties of relativistic charged particles and free space through its definition

$$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx 0.0072973525693 \qquad (1)$$

where e is the elementary charge, $\hbar$ is the reduced Planck constant, c is the speed of light, and ε_0 is the vacuum electric permittivity. Equation 1 imposes constraints on the allowed values of certain elemental constants depending on the employed system of units. For example, in atomic units widely utilized in atomic, molecular, and materials physics, $\hbar = e = 4\pi\varepsilon_0 = 1$, implying that $c = \alpha^{-1}$. In natural units, often used in quantum field theory, $\hbar = c = \varepsilon_0 = 1$; hence, $e = \sqrt{4\pi\alpha}$. In quantum electrodynamics, α is used as a small parameter for perturbative corrections in calculations of field−matter interactions, which are typically expressed as a quickly convergent series in terms of powers of α. In contrast, in atomic, molecular, and materials physics, α appears explicitly only rarely. When it does, it is considered a scientific breakthrough, as prominently illustrated by the seminal example of visual transparency of graphene, determined solely in terms of α.[3,4] Let us consider a general form of the nonrelativistic Hamiltonian for a nucleo-electronic system

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_i}\nabla_{\mathbf{r}_i}^2 + \frac{1}{2}\sum_i\sum_j \frac{q_i q_j}{4\pi\varepsilon_0|\mathbf{r}_i - \mathbf{r}_j|} \qquad (2)$$

where m_i is the mass of ith particle, $\mathbf{r}_i$ its position, and q_i its charge. Obviously, FSC does not explicitly appear in this formula. Formally, one can introduce the FSC by using its definition in eq 1 and rewriting the Coulomb potential as $\frac{q_i q_j}{4\pi\varepsilon_0|\mathbf{r}_i - \mathbf{r}_j|} = \frac{\alpha\hbar c(q_i / e)(q_j / e)}{|\mathbf{r}_i - \mathbf{r}_j|}$. However, this awkward-looking expression is not used in practice since in nonrelativistic quantum mechanics $c \to \infty$; hence, α can be assumed to vanish.[5] Similarly, the FSC does not appear in calculations of response properties of material systems. For example, the static (infinite-time) polarizability of a nucleo-electronic system $\mathcal{A}(\omega = 0)$, describing the interaction between the electric field and matter, is given in terms of ground and excited states of the Hamiltonian in eq 2 as[6]

$$\mathcal{A} = \frac{2}{3}\sum_{n\neq 0}^{\infty} \frac{\langle\Psi_0|\hat{\mathbf{d}}|\Psi_n\rangle\cdot\langle\Psi_n|\hat{\mathbf{d}}|\Psi_0\rangle}{E_n - E_0} \qquad (3)$$

where Ψ_n is the wave function of the nth state of the system and E_n is its energy, whereas $\hat{\mathbf{d}} = \sum_i q_i\hat{\mathbf{r}}_i$ is the electric dipole operator. In practice, the evaluation of this formula is difficult even for isotropic multielectron atoms, whose ground-state wave function is already characterized by a multitude of

orbitals with different principal, angular, and magnetic quantum numbers. In addition, eq 3 involves a sum over all bound and continuum excited states. Here, we provide an alternative view on the electronic polarizability by predicting its value for atoms from their geometric van-der-Waals (vdW) radii through α. In doing so, the relevance of FSC in atomic and molecular physics is extended from acting as a small perturbative parameter for field−matter interactions to directly determine electronic properties of atoms.

We start by establishing an empirical connection between the electronic polarizability of atoms and α and then proceed to a phenomenological derivation from the perspective of interacting matter and field. Two radically different scaling laws can be employed for expressing the atomic polarizability as a function of two effective atomic length scales[7−9]

$$\mathcal{A}_{cl} = 4\pi\varepsilon_0 R_{cl}{}^3, \qquad \mathcal{A}_q = \frac{4\pi\varepsilon_0}{a_0{}^4}\Phi^{-7}R_{vdW}{}^7 \qquad (4)$$

The classical scaling law for $\mathcal{A}_{cl}$ stems from a conducting spherical shell[7] or a hard sphere with uniform electron density surrounding a positive point charge,[8] whereas the quantum scaling law for $\mathcal{A}_q$ stems from the balance between exchange and correlation forces between two closed-shell atoms.[9] The dimensionless constant $\Phi = 2.54 \pm 0.02$ has been obtained empirically in ref 9 by fitting the relation between atomic polarizabilities and vdW radii derived for noble gases from experimental scattering and crystal-structure data, respectively.

From eq 4, there exists a critical radius R_c, such that $R_{cl} = R_{vdW} = R_c$, for which $\mathcal{A}_{cl} = \mathcal{A}_q = \mathcal{A}_c$. Imposing the first condition and solving for the second, we obtain

$$R_c = (5.11 \pm 0.07)a_0, \qquad \mathcal{A}_c = 4\pi\varepsilon_0(133.5 \pm 5.5)a_0{}^3 \qquad (5)$$

For the moment, it is plausible to explore the implications of setting the value of $\mathcal{A}_c$ equal to the inverse of the fine-structure constant, $\mathcal{A}_c = \alpha^{-1} \approx 137.036$, in atomic units (au). Consequently, $R_c = \alpha^{-1/3}a_0 \approx 5.156a_0$, and hence the second formula in eq 4 can be written as

$$\mathcal{A}_q = \frac{4\pi\varepsilon_0}{a_0{}^4}\alpha^{4/3}R_{vdW}{}^7 \qquad (6)$$

The numerical prefactor $(\alpha^{4/3})^{-1/7} \approx 2.553$, with an unusual fractional power of α, falls well within the statistical interval 2.54 ± 0.02 determined for atoms in ref 9. The accuracy of eq 6 is also convincingly demonstrated in Figure 1 by comparing vdW radii obtained from electronic polarizabilities to their reference values independently determined from experimental crystal data for interatomic vdW contacts. The potential connection between the second formula in eq 4 and the fine-structure constant is remarkable, because $\mathcal{A}_q$ was derived from a model of two interacting neutral atoms, while α measures the interaction strength between photons and charged particles. Of course, any interaction between atoms is propagated by the underlying vacuum field and in what follows we propose a phenomenological model for $\mathcal{A}_q$. A first-principles derivation for $\mathcal{A}_q$ would require nonperturbative quantum electrodynamics (QED) for atomic bound states, as given by quantum canonical transformations,[10,11] computational methods,[12,13] or a variational formulation of QED.[14,15]
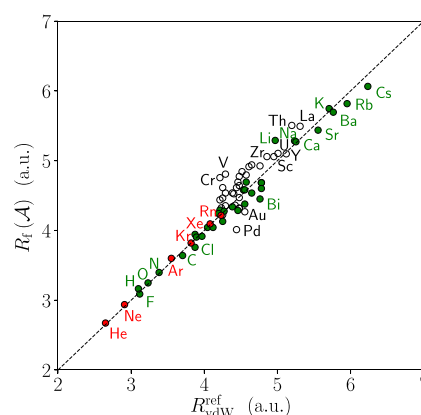

Figure 1. Comparison between literature values for van-der-Waals radii, R_{vdW}^{ref}, from the experimental data of refs 16 and 17 and field radii R_f obtained by means of eq 13 for 72 atoms in the periodic table. For this plot, atomic polarizabilities calculated from first-principles in ref 18 were used and all quantities are presented in atomic units. The noble gases and the transition metals are indicated by red and empty dots, respectively. All other elements including nonmetals and simple metals are shown with green dots.

All these nonperturbative QED methods are still undergoing development, which is why we resort to phenomenology.

The remarkably accurate and simple relation between electronic polarizability and atomic vdW radius, eq 6, becomes demystified by realizing the fact that α, defined by eq 1, can be understood as a ratio between two polarizability densities

$$\alpha = \frac{e^2/\hbar c}{4\pi\varepsilon_0} \qquad (7)$$

By its definition in eq 4, the vacuum permittivity ε_0 has units of polarizability density. Since the FSC is a dimensionless quantity, $e^2/\hbar c$ also has units of polarizability density by virtue of combining three fundamental physical properties: elementary charge, Planck's constant, and the speed of light.

The FSC measures the interaction strength between charged particles and the electromagnetic field, whereas the polarizability density $\bar{\mathcal{A}}$ determines local energy density when multiplied by the local electric field squared.[6] Similar to atoms and molecules where electric polarization arises via formation of permanent or transient electric multipoles, the QED vacuum (i.e., the photon field dressed by particle/antiparticle quantum fluctuations), can be characterized by a finite polarizability density.[19,20] In addition, matter (an atom in our consideration) perturbs the QED vacuum by causing a cloud of virtual photons surrounding the atom.[21−25] Throughout this paper we use the term "field" either for the free-space photon field or its modified state due to a cloud of virtual photons, as a local perturbation of the QED vacuum by the presence of an atom possessing spherical symmetry with respect to the atomic nucleus.

The aforementioned facts suggest the following interpretations for α

$$\alpha = \frac{\bar{\mathcal{A}}_f}{\bar{\mathcal{A}}_m} = \left.\frac{V_m}{V_f}\right|_{\mathcal{A}_f=\mathcal{A}_m} = \left.\frac{R_m{}^3}{R_f{}^3}\right|_{\mathcal{A}_f=\mathcal{A}_m} \qquad (8)$$

where degrees of freedom of matter (atom) and fields are labeled by m and f, respectively, $\bar{\mathcal{A}}_{m(f)}$ is the polarizability density of matter (field), and $V_{m(f)}$ represents the polarized

radial volume of matter (field) in the presence of electromagnetic field (matter). The conditions defined by the two last identities in eq 8 can be interpreted in the following way. The FSC is the ratio between the effective volume V_m of an atom and the volume V_f of a sphere surrounding this atom such that the cloud of virtual photons induced by the presence of matter has its polarizability $\mathcal{A}_f$ equal to the atomic polarizability $\mathcal{A}_m$. The latter condition is imposed according to the energy conservation of the combined atom/field system since energy is directly proportional to the polarizability.[6]

The classical polarizability expression, given by the first formula in eq 4, does not contain any relation between the constant field polarizability density $4\pi\varepsilon_0$ and the classical hard-sphere polarizability radius R_{cl}. Obviously, matter and field are mutually interacting and hence the classical formula needs to be replaced by $\mathcal{A}_m = \bar{\mathcal{A}}_m(R_m)R_m{}^3$ for the quantum-mechanical consideration. However, it is easier to tackle the problem from the field perspective, by employing the aforementioned condition of the energy conservation. Then, one can write a general expression for an interacting polarizability as

$$\mathcal{A}_m = \mathcal{A}_f = \bar{\mathcal{A}}_f(R_f)R_f{}^3 \tag{9}$$

where R_f is a certain field polarization radius that connects with the field polarizability density $\bar{\mathcal{A}}_f(R_f)$. Inspired by quantum electrodynamics, we assume that an atom excites a single effective harmonic-oscillator mode of the field with the length scale R_f. The field polarizability density can be then expressed as[18,26,27]

$$\bar{\mathcal{A}}_f(R_f) = 4\pi\varepsilon_0\left(\frac{R_f}{R_f^0}\right)^4 \tag{10}$$

where R_f is the Gaussian wave function spread of the spherically symmetric field oscillator and $(R_f^0)^4$ is a four-dimensional volume normalization factor. Equation 10 states that the average polarizability density of the dressed photon field scales quartically with respect to the radius of the sphere (centered on the atomic nucleus) over which the field properties have been averaged. Such a modification of the field polarizability density is due to the presence of the atom that causes a renormalization of the bare value $4\pi\varepsilon_0$ valid in the absence of matter. The local change of field properties is caused by the cloud of virtual photons surrounding the corresponding atom.[21−25]

To determine R_f^0, we connect the length scales R_m, R_f and polarizability densities $\bar{\mathcal{A}}_m$, $\bar{\mathcal{A}}_f$ of matter and field by using the two interpretations of α in eq 8. We first note that a homogeneous sphere of matter with a radius $R_m = a_0$ should have its polarizability density given by $\bar{\mathcal{A}}_f = 4\pi\varepsilon_0$, according to eq 9. Using the definitions in eq 8 yields $R_f = \alpha^{-1/3}a_0$ and $\bar{\mathcal{A}}_m = 4\pi\varepsilon_0\alpha^{-1}$. With these length scales and polarizability densities we now use the condition $\mathcal{A}_f = \mathcal{A}_m$ employed to define the right-hand side of eq 8. This yields the following identity

$$4\pi\varepsilon_0\alpha^{-1}a_0{}^3 = 4\pi\varepsilon_0\left(\frac{\alpha^{-1/3}a_0}{R_f^0}\right)^4\alpha^{-1}a_0{}^3 \tag{11}$$

from where we determine $R_f^0 = \alpha^{-1/3}a_0$. Thus, the normalization radius R_f^0 in eq 10 corresponds to the critical radius R_c of eq 5 (also see discussion after this equation).

Inserting this value of R_f^0 into eqs 9 and 10 leads to the final equation for the polarizability

$$\mathcal{A}_m = \frac{4\pi\varepsilon_0}{a_0{}^4}\alpha^{4/3}R_f{}^7 \tag{12}$$

which agrees with eq 6 when setting $R_f = R_{vdW}$. This suggests that R_{vdW}^A is the effective length scale of an excited field oscillator for an atom A.

Using eq 12, we can now calculate R_f for any atom in the periodic table given its polarizability $\mathcal{A}_m$ as

$$R_f(\mathcal{A}_m) = \left(\frac{\mathcal{A}_m a_0{}^4}{4\pi\varepsilon_0}\right)^{1/7}\alpha^{-4/21} \tag{13}$$

Figure 1 shows the values of $R_f(\mathcal{A}_m)$ obtained from eq 13 using atomic polarizabilities $\mathcal{A}_m$ corresponding to linear response coupled cluster quantum-chemical calculations,[18] plotted versus the experimental reference data for vdW radii of 72 atoms from refs 16 and 17. Accurate atomic polarizabilities and vdW radii are known for the noble gases. In this case, the vdW radius is simply defined as half of the equilibrium distance in a homoatomic dimer. Indeed, we observe an excellent agreement between R_f and R_{vdW}^{ref} in Figure 1 for these atoms. A similar situation is found for all organic elements in the periodic table. For other atoms, reference vdW radii have increased statistical uncertainties,[16] since vdW radii are determined from the experimentally measured molecular crystal structures. For the purpose of estimating atomic vdW radii, every molecule is considered as its own spin-compensated entity. The closest interatomic distances between atoms on neighboring molecules, interacting through vacuum, serve to define a set of values for atomic vdW radii. Owing to the statistical nature of vdW radii determined from crystal structures, higher uncertainties are expected for the transition metals possessing various spin states in crystalline compounds. This is the most likely reason for the increased deviations between R_f and R_{vdW}^{ref} obtained for Cr (12.88%) and V (12.07%). However, the average relative error for all 72 elements shown in Figure 1 is just 3.07% and it reduces to 0.05% by restricting our consideration to the noble gases only.

An interesting application of eq 12 is the possibility to obtain α or its inverse, which is numerically equivalent to the speed of light in atomic units, by means of nonrelativisic quantum-mechanical calculations. One just needs to determine the atomic polarizability $\mathcal{A}_m$ and the equilibrium interatomic distance $R_{eq} = 2R_{vdW}$ in homonuclear vdW-bonded dimers. Both quantities can be computed reliably from state-of-the-art quantum-chemical methods for closed-shell atoms. The resulting prediction of α^{-1} is shown in Table 1 for the six noble gases from He to Rn. The atomic polarizabilities and equilibrium internuclear distances have been obtained from high-level calculations based on linear response coupled cluster (CC) theory[18] and CC with single, double, and perturbative triple excitations [CCSD(T)] calculations for binding energy curves.[30−32] The computed values R_{vdW}^{calc} do not account for nuclear quantum vibrations, particularly important for the He dimer. For this reason, in Table 1 we also provide comparative

Table 1. Estimation of α^{-1} (Numerically Equivalent to the Speed of Light in Atomic Units) from Nonrelativistic[28] Quantum-Mechanical Calculations on Noble Gas Atoms and Their Homonuclear Dimers[29]

species	$\mathcal{A}_m$	R_{vdW}^{calc}	R_{vdW}^{exp}	$\alpha^{-1}(R_{vdW}^{calc})$	$\alpha^{-1}(R_{vdW}^{exp})$
He	1.38	2.81	2.65	178.16	130.96
Ne	2.67	2.92	2.91	132.85	130.48
Ar	11.10	3.56	3.55	129.16	127.26
Kr	16.80	3.82	3.82	137.04	137.04
Xe	27.30	4.11	4.08	139.81	134.54
Rn	33.54	4.18	4.23	130.92	139.35

estimates of α^{-1} obtained using the experimentally determined vdW radii. Both estimates of the FSC are in good agreement, except for a significant deviation observed for He, owing to large nuclear quantum effects contributing to the experimental R_{vdW}^{exp}, but missing from electronic *ab initio* calculations. We remark that Kr is the only atom for which the experimental and calculated R_{vdW} values coincide, and it is here that the estimated $\alpha^{-1} = 137.04$ is in perfect agreement with its well-known reference value $\alpha^{-1} \approx 137.036$.[1,33−35] The small uncertainty in the calculated values of the polarizabilities and the vdW radii for noble gases is not the only reason for the observed discrepancy. It is also possible that the formula given by eq 6 corresponds to a leading-order approximation. Higher-order terms with respect to the FSC might need to be considered for furnishing a more accurate formula. This implies a need to develop detailed microscopic models describing intrinsic vacuum response properties.[36,37] A derivation of eq 6 could also be accomplished by generalizing a model describing a cloud of virtual photons surrounding a many-electron atom.[21−25]

In summary, we presented a heuristic derivation of the relation between electronic polarizability of atoms with their geometric vdW radii through the fine-structure constant. The formula provided by eq 13 has a 3% average accuracy for estimating vdW radii of 72 atoms compared to reference data obtained from experimental crystal structures. However, more work is required to derive a first-principles connection between R_f and R_{vdW}, without the empiricism used here, and the unsolved problem of nonperturbative QED treatment of coupled many-electron atoms and field. For example, we suggest that R_f can be defined as an operator acting on the field−matter wave function and it is coupled to R_{vdW} through the force balance between quantum exchange and correlation forces.[9] Our derivation extends the influence of the FSC from quantum electrodynamic effects and optical properties of low-dimensional materials to atomic response properties throughout the periodic table of elements.

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Notes
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