Quantum-mechanical relations between polarizabilities and geometric properties of atoms

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Many properties of real physical systems can be captured by approaches based on Gaussian wave functions. Among them, the quantum Drude oscillator (QDO) model [1–3] serves as an insightful and efficient approach for the description of atomic response properties as well as van der Waals (vdW) interactions. Within this model, all valence electrons in an atom are represented by a single *Drude particle* characterized by its charge, mass, and characteristic frequency. The Gaussian wave function of the QDO allows to perform analytical derivations of the atomic properties related to vdW interactions, which fulfill several scaling laws valid for real atoms. Particularly, invariants constructed from the dispersion coefficients or the atomic polarizabilities within the QDO model accurately capture real atomic properties [3]. Recently [4–5], this model helped to unveil the non-trivial relation between the dipole polarizability and the atomic volume, $\alpha_{\text{dip}} \propto V^{4/3}$. We have also discovered a very surprising relationship between the multipole polarizabilities and the vdW radius as well as the equilibrium distances in vdW-bonded atomic dimers [6]. Here, we give an overview of all these remarkable findings and show their impact on practical applications. In particular, the parametrization of interatomic vdW potentials becomes now easier due to the obtained quantum-mechanical relations between the polarizability and the equilibrium distances in homonuclear as well as heteronuclear dimers. This reduces the empiricism and improves the accuracy of corresponding approaches. The revealed relations also allow to amend the scheme for evaluating the effective atomic radius in a molecule, which improves the accuracy of computational models for intermolecular interactions like the Tkatchenko-Scheffler method [7].

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