**GROUND AND EXCITED STATE MOLECULAR POLARIZABILITY**

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Dipole polarizability α(ω) is a fundamental molecular property describing the response of the electrical charge distribution to an external electric perturbation. Its primary importance arises from its role in the description of molecular interactions, scattering processes, foundations of optical spectroscopy *e.g.* [1]. General expression for the dipole polarizability clearly indicates that it is a complex tensor quantity:

The real static part of α(0) can be computed at the very high level of approximations, *i.e.* CCSD(T) or CC3, nowadays, almost routinely.

Much less is known about polarizability of excited states, and dynamic polarizability for frequencies close to the electronic resonances. In the first part of the presentation the simple approach combining standard TDDFT calculations and the well-known numerical differentiation technique is shown to yield accurate results for the low-lying excited states of small organic molecules like uracil etc. For determination of the dynamic polarizability of the excited states we employed the damped response theory [2] applied to the CASSCF wavefunction. The results for the Rydberg-like singlet and triplet states of H2O and H2S are very encouraging, strongly confirming the usefulness of our approach. Finally, we tested the reliability of very simple DFT-based computations of the polarizability tensor α(iω), i.e. the polarizability for the imaginary frequencies. This property is necessary for the determination of C6 coefficient, the leading term in the long-range expansion of the dispersion energy. The results for closed-shell atoms like Ar or Mg are very accurate, while the case of Be needs the proper CASSCF wavefunction to take into account the near degeneracies.

REFERENCES

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