Recent developments in the determination of molecular properties

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A few recent achievements within the area of the accurate determination of molecular (response) properties will be discussed.
Among these, a novel atomic-orbital based formulation of response theory [1,2] currently under implementation within a local version of the Dalton program [3] will be presented. Test results for excitation energies and linear response properties, excited state first order properties as well as excited state gradients will be given.
The results of a statistical study on the accuracy of standard ab initio methods in the determination of molecular geometries of systems containing second row atoms will also be discussed [4].

References

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[3] DALTON, a molecular electronic structure program, Release 2.0 (2005), see http://www.kjemi.uio.no/software/dalton/dalton.html

[4] S. Coriani, D. Marchesan, J. Gauss, C. Hättig, T. Helgaker, P. Jørgensen. Submitted to J. Chem. Phys.