Calculation of magneto-electric birefringences

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In our contribution we present the first study of relativistic effects on the electric-field-gradient-induced birefringence (Buckingham birefringence) for the series of molecules CX_2 (X=O, S, Se, Te). Using the OpenRSP [1] and XCFun [2] libraries we extend a recently presented atomic-orbital-driven scheme for the calculation of time-dependent molecular properties using one-, two- and four-component relativistic wave functions [3]. to include frequency-dependent magnetic field perturbations to first order, using London atomic orbitals to ensure gauge origin independence of the calculated results. Results are presented both at the Hartree–Fock and Kohn–Sham density functional level of theory.

[1] A. J. Thorvaldsen, K. Ruud, K. Kristensen, P. Jørgensen, S. Coriani, *J. Chem. Phys.* **129**, 214108 (2008).

[2] U. Ekström, L. Visscher, R. Bast, A. J. Thorvaldsen, K. Ruud, *J. Chem. Theory Comput.*, **6**, 1971 (2010).

[3] R. Bast, A. J. Thorvaldsen, M. Ringholm, K. Ruud, *Chem. Phys.* **356**, 177 (2009).