Calculating vibrational contributions to molecular electric and magnetic properties

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In this talk, I will discuss our recent work on developing analytic methods for calculating vibrational effects on electric and magnetic properties calculated using self-consistent field (SCF) wave functions, including Hartree-Fock and Kohn–Sham density functional theory [1]. Particular attention will be given to calculating higher-order derivatives of exchange-correlation kernels using automatic differentiation [2], including corrections from magnetic field or geometry dependence in the basis set. The extension of the formalism to calculating excited-state properties will also be addressed.
Different applications of the code will be presented, including calculations of Coherent Anti-Stokes Raman Scattering [3,4], pure vibrational corrections to nonlinear hyperpolarizabilities [5], as well as recent work on the vibronic effects in the Magnetic Circular Dichroism spectrum of ethylene [5].

Literature:

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