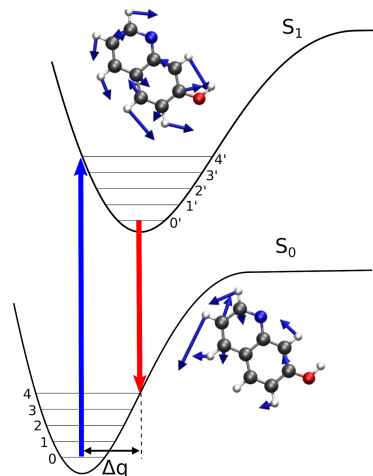


## Excited-State Properties from Analytic TDDFT Hessians

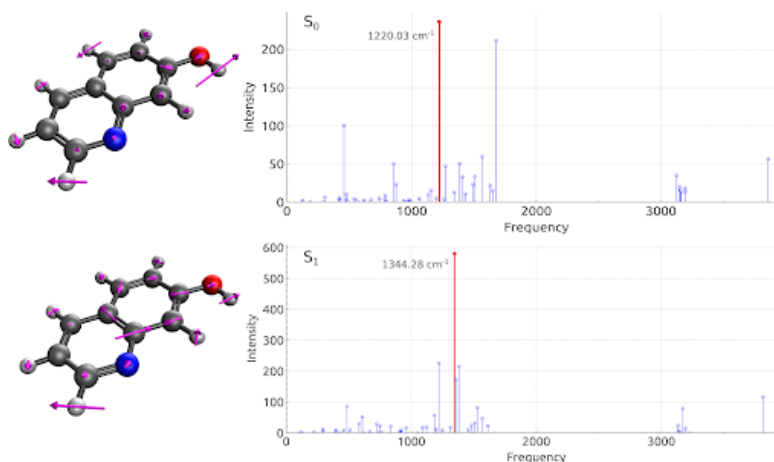
**Analytic TDDFT Hessians are available for a wide range of modern exchange-correlation functionals including meta-GGAs:**

- Much less costly than post-HF methods such as CASSCF and CC and thus applicable to larger molecules.
- Analytic Hessians are more efficient than numerical derivatives in geometry optimization. Excited-state geometry optimization can be more robust.
- Searching for critical points on excited-state potential surfaces is more robust with analytic Hessians.



**Applications involving TDDFT Hessian calculations:**

- Excited-state geometry optimizations and potential energy scans.
- Excited-state frequency calculations, time-resolved IR analysis.
- Fluorescence and phosphorescence, photochemistry and photophysics.
- Vibrationally resolved electronic spectroscopy simulation.
- Resonance Raman spectroscopy simulation.



Excited-state frequency analysis with meta-GGA xc functional MN15-L

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