SI2-SSI: Chronus Quantum (ChronusQ) - Sustainable Open-Source Quantum Dynamics and Spectroscopy Software

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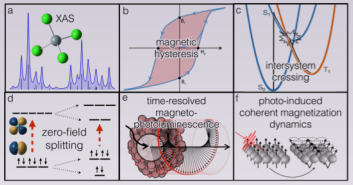
Functionality Highlights

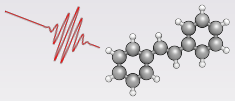
Interaction between matter and electromagnetic radiation can be modeled from first-principles using time-dependent quantum mechanics. Properties can be computed to provide molecular insights to experiment.

Spectroscopic Properties

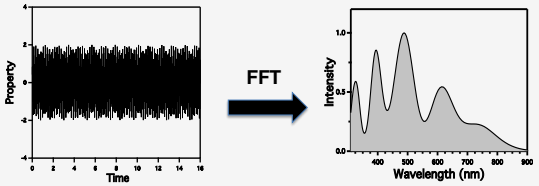
ChronusQ provides convenient modules to evaluate a number of properties which are important to the field of spectroscopy.



Time-Dependent Electronic Structure

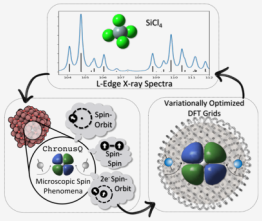


A primary component of ChronusQ is a high-performance and robust integrator for the time-dependent Schrodinger and Dirac equations. Time integration in the presence of an arbitrary number of fields of various character and amplitude envelopes is supported. For a given perturbation, evaluation of a full suite of electronic properties allows for simplified access to spectroscopic properties in the time and frequency domains. Prebuild modules for the linear absorption and electric circular dichroism are provided.



Relativistic Electronic Structure Theory

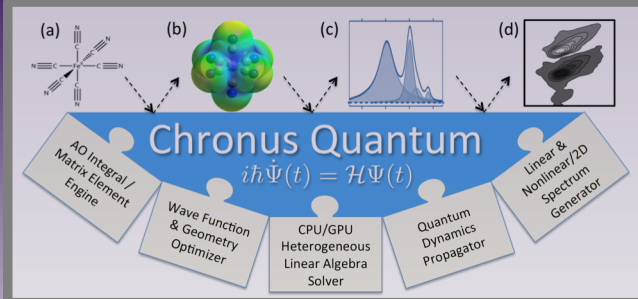
Relativistic electronic structure theory is required to accurately treat heavy-elements and simulating many important phenomena such a spin-orbit coupling, the inert pair-effect, and spin-forbidden reactivity. ChronusQ provides an implementation of the exact two-component (X2C) relativistic method using both Hartree-Fock and Kohn-Sham wave functions.



Obtaining ChronusQ

ChronusQ is open source and released under GPLv3

- http://www.chronusquantum.org
- http://github.com/liresearchgroup/chronusq_public

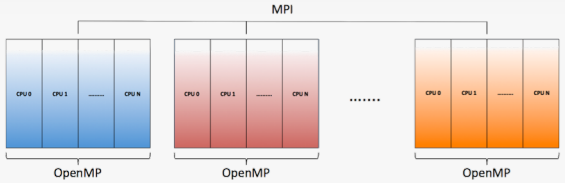


Technical Highlights

The following depicts a number of technical highlights within the ChronusQ software package.

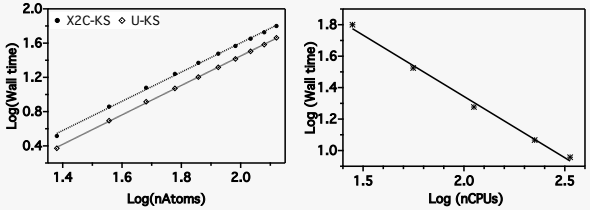
Hybrid OpenMP + MPI Parallelism

ChronusQ utilizes a hybrid parallelism scheme which exploits shared memory parallelism (OpenMP) on a single compute node and MPI across compute nodes to minimize data communication.



Scalable Relativistic Density Functional Theory

ChronusQ implements a scalable algorithm for the treatment of non-collinear relativistic density functional theory using torque free auxiliary variables. [3]



Exploitation of Fast Quaternion Arithmetic in Relativistic Calculations

ChronusQ has integrated the HAXX software infrastructure [5] to exploit quaternion arithmetic in closed shell relativistic calculations

HAXX

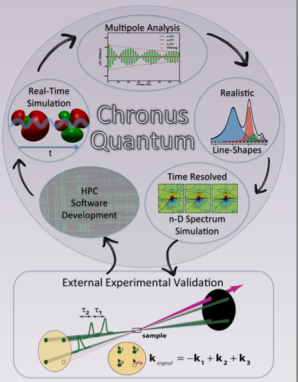
Future Development

Time-Resolved Spectroscopy

- ❑ Transient Infrared Spectroscopy
- ❑ Transient UV/Vis Spectroscopy

Furthering Relativistic Electronic Structure Theory

- ❑ Development of all-electron atomic centered basis sets for heavy elements



- ❑ Extension of two-component relativistic methods to include two-electronic spin-couplings

Magnetic Field Perturbations

- ❑ Magnetic spectroscopic properties in time and frequency domains
- ❑ Gauge including atomic orbitals (GIAOs)

ChronusQ Publications

[1] Van Beeumen, R.; Williams-Young, D.B.; Kasper, J.; Yang, C.; Ng, E.; Li, X.; *J Chem. Theory Comput.* **2017**, 13(10), 4950-4961

[2] Lestrange, P.; Williams-Young, D.B.; Jimenez–Hoyos, C.; Li, X.; *J. Chem. Theory Comput.*, **2018**, 14(2), 588–596.

[3] Petrone, A.; Williams-Young, D.B.; Sun, S.; Stetina, T.; Li, X.; *Eur. J. Phys. B.* **2018**. Submitted.

References

[4] Li, X.; Valeev, E.; Williams-Young, D.B.; Petrone, A.; Goings, J.J.; Ding, F.; Liu, H.; Sun, S.; Lestrange, P.; *Chronus Quantum*, Beta 1. **2018.**

[5] Williams-Young, D.B.; *HAXX: Hamilton's Quaternion Algebra for C++.* https://github.com/wavefunction91/HAXX

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