Implementation of CW-EPR, A Python Program for Analyzing and Processing EPR Spectra

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Abstract

The need for reproducibility at the heart of science led to the necessity of modular user interface with the advent of computer-based data processing and analysis. Dr. Bill Tiskup and Dr. Mirjam Schroder designed CW-EPR, a python program that allows for EPR spectra to be reproduced with little to no coding skills required. The H-SC Chemistry Department showed desire to use this program for analyzing and processing raw EPR data in a classroom setting. The program needs to read specific files used by the Chemistry Department, including DAT and LMB files.

Introduction

Electron Paramagnetic Resonance (EPR) Spectroscopy (also known as Electron Spin Resonance (ESR) Spectroscopy) is an analytical technique used to detect unpaired electrons or free radicals in a compound. The basis of EPR spectroscopy comes from the spin of an electron and its magnetic moment. When applied in a magnetic field the two possible spin states of the electron have two different energies. It demonstrates the concept of the Zeeman effect because lower energy states occur when the spin is aligned with the magnetic field and higher energy states occur when the spin is aligned against the magnetic field. When radiation is being absorbed it is presented as a first derivative on a graph. Unpaired electrons are also sensitive to local environment which causes a magnetic field within nuclei resulting in hyperfine splitting. Hyperfine splitting provides valuable information regarding the identity and number of nuclei as well as detecting unpaired electrons.

Literature Review

Dr. Bill Tiskup and Dr. Mirjam Schroder discuss the need for easier reproducibility of raw data necessary to simulate spectra. The article heavily emphasizes the necessity of reproducibility as a fundamental of science as well as source of development for the survival of mankind. Computer programming was used to create a simple user interface designed to ease analyzing and processing raw data to accurately simulate spectra from previous publications.

Continuous Wave Electron Paramagnetic Resonance (CW-EPR) Spectroscopy is a type of EPR spectroscopy that records samples via a field of constant frequency and an external field sweep until resonance conditions are met. CW-EPR was the best candidate for the project because of its ability to record samples at room temperature and detect most paramagnetic species. The program is designated as CWEPR and uses Python as its preferred programming language.

Method

The H-SC Chemistry Department desires to use the interface in a classroom setting as well as simulating raw data of EPR spectra in LMB and DAT file formats. The chemistry lab has previously used WINSIM 2002 as the software used to simulate spectra, but now wants a program that can be used with little to no knowledge of coding. *Science Computing for Chemists* was an easy source used to learn basic Python programming. CWEPR.de provides excellent documentation on the program itself including what it does and how it works. Collaboration with Dr. Bill Tiskup was necessary in order to simulate EPR spectra using similar Bruker file formats used in the Chemistry Department.

Results

CWEPR is dependent on recipe-driven data analysis**,** which requires a recipe for Python to “cook” in order to process the available raw data. The “recipes” are written using the YAML programming language, which is a human readable computer language that relies heavily on strings, numerical values, and Boolean values. Visual Source Code was used to write and edit YAML files for “recipes”. Once the raw data and “recipe” are completed, they are to be inputed in Python and using the “serve” command, to “cook” the “recipe”. The Python package includes multiple modules used in each step of the ”recipe”. These modules are used for analyses, datasets, exceptions, metadata, plotting, processing, reporting, and utilities.

Conclusion

CWEPR was successful in simulating EPR spectra within the LMB and DAT formats and can easily be operated by a student with little to no programming skills. The YAML recipes may be tedious to complete and write due to the number of steps required for Python to read the raw data but is easy to complete because of the YAML programming language. Python and Visual Studio Code are the tools needed for simulating EPR spectra and the module CWEPR needs to be installed within python before any other step. The program has the potential to simulate numerous EPR spectra located within the Chemistry Department. A student manual will also accompany the Chemistry Department for faculty/students to use for help in the situation where programming errors are faced or CWEPR is performing the wrong task.

Acknowledgements

I want to give my thanks to the H-SC Chemistry Department for providing the necessary equipment for my research as well as my advisor Dr. Herbert J. Sipe, Jr. I also want to give thanks for the H-SC Summer Research program for providing housing for on-campus research and funding as well as Dr. Michael Wolyniak for managing research presentations.

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