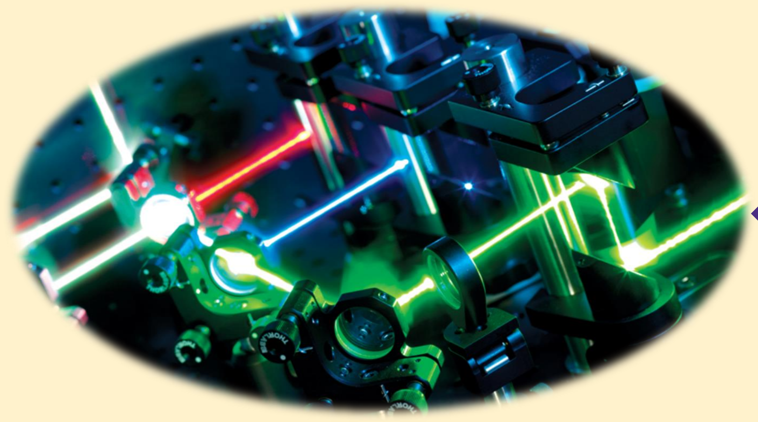

Peakaboo

Self-Consistent Identification of Spectral Signatures in Transient Absorption Spectroscopy

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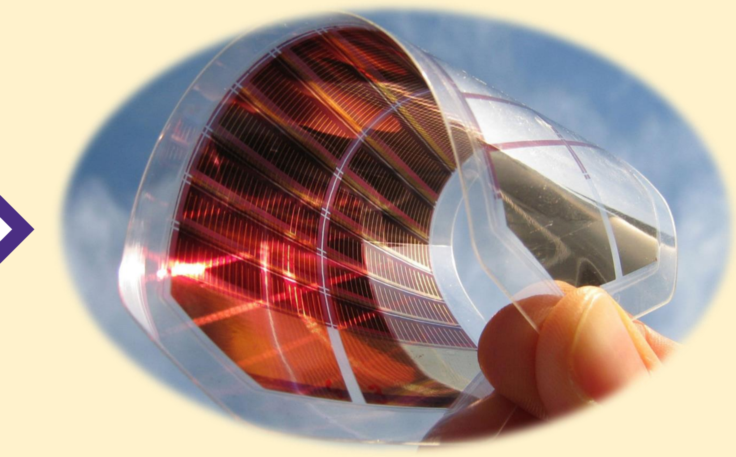
Sponsored by Prof. David Ginger



Motivation

Transient absorption (TA) spectroscopy is a crucial tool for understanding the dynamics and efficiency of charge carrier generation and recombination in photovoltaic materials. In a typical two-way TA spectrum, the observed signal is convoluted by contributions from multiple populations. Each species contribution has unique spectral signatures and dynamics, and evolve differently over time. Further, the signals observed are unique to each material system, which impedes traditional means of assigning *x* spectral signature to *y* species/process. Thus requiring each TA spectrum to be individually evaluated, which creates a bottleneck in the feedback loop of material development and characterization.

Herein, we demonstrate an open-source data analytics package to *self-consistently* identify, differentiate, and visualize temporally evolving signatures of distinct species

Workflow

>>> load_data

User inputs raw data collected from experiment; our parser separates the data into arrays of time, wavelength, and intensity

>>> data_smoothing

Noisy raw data is smoothed by multivariate spline fitting[1]

>>> find_peaks

Peaks are found by a gradient based differential calculation,[2] the peak index, intensity, and probable full-width half-max are recorded

>>> peak_classify

Peaks from the same feature are grouped together by predictive data clustering[3]

>>> feature_visualizer

Peak intensity and position is visualized to show spectral evolution over time

>>> kinetics_fitting

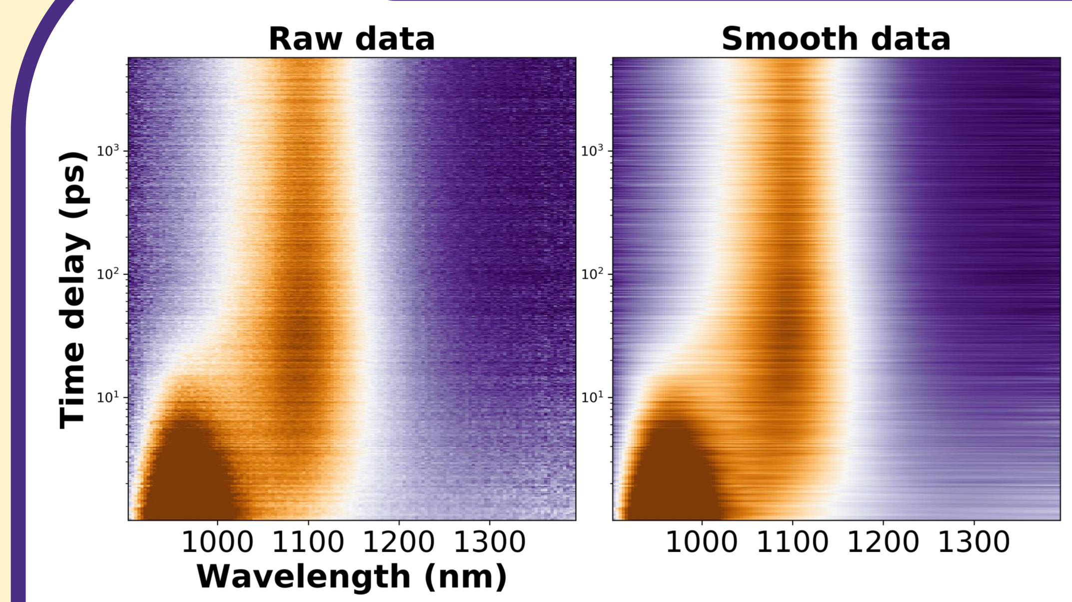
Excited state lifetimes are calculated by fitting exponential functions to intensity growth/decay

References

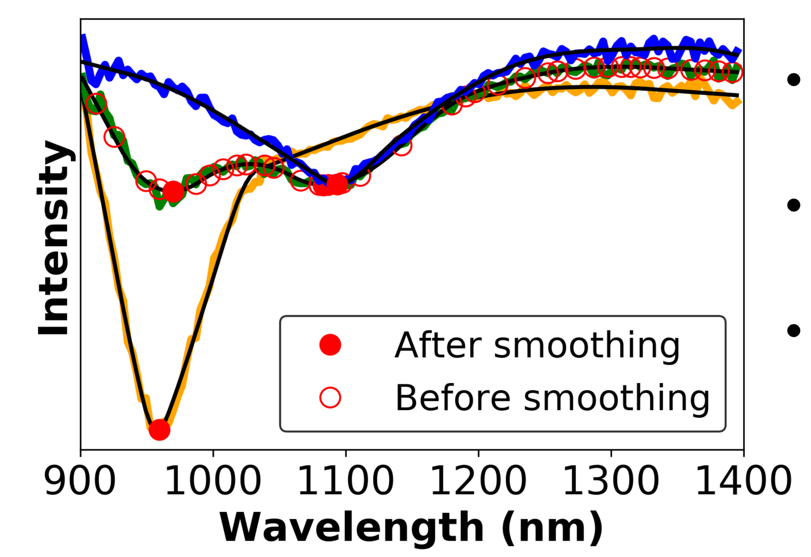
Open Source Packages Used

1. Py-Earth 2. PeakUtils 3. Sklearn.clusters

Data Smoothing and Peak Finding



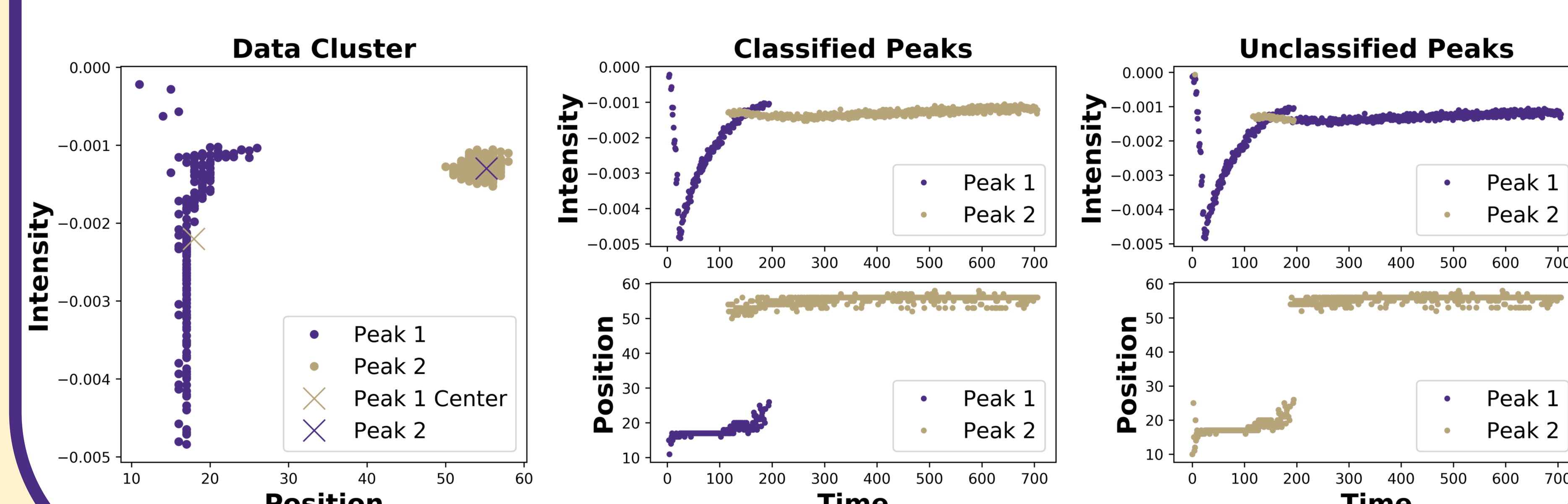
- Transient absorption spectra are inherently noisy
- Noise makes it more difficult to accurately interpret spectral features and identify peaks
- We smooth these spectra with a multivariate adaptive regression spline fitting function



- Our peak finding function is based on a gradient differential calculation
- Spectra smoothing drastically increases accuracy in identifying peaks
- This combination allows for good peak detection with minimal external input

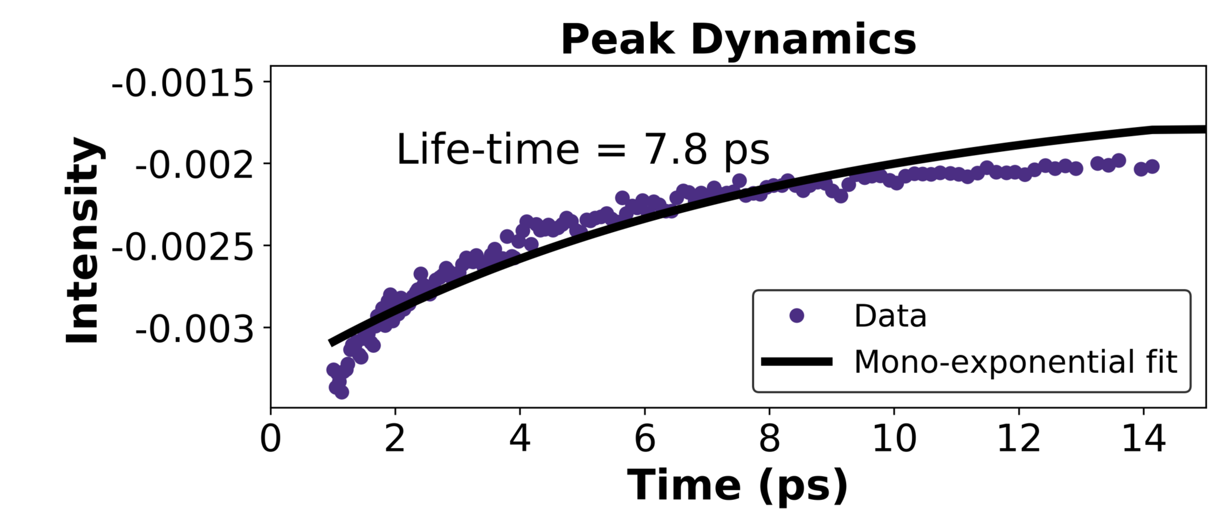
Peak Classification and Visualization

- Peaks identified by the peak finding algorithm are classified based on their similarity to other peaks found at other points in time
- The K-means clustering method solves for the minimal variance between peak descriptors when confined to *k* number of peaks
- Classifying peaks by this method is a crucial component of separating the signal detected from the many species observed at a given time



Kinetics Fitting

- Once species are separated, we determine their lifetime by fitting the change in intensity to an exponential function
- This provides the user with valuable information about the photophysical properties of the materials



Future Work

>>> improved_peak_finding

Develop algorithm to iteratively fit a mixture of regular line shapes to the smooth spectra. By finding a fit with minimum error we hope to elucidate the presence of peaks that cannot be detected by our current functions

>>> improved_peak_classification

By defining peaks with entire line shapes, rather than 2D descriptors, we hope to improve the accuracy of peak classification by methods like dynamic time warping

>>> improved_feature_visualizer

Develop user interactive visualization of specific line shape evolution overtime

>>> improved_kinetics_fitting

Expand the functions with which we can fit feature kinetics, as not all species can be fit by a single exponential growth/decay

>>> improved_feedback_loop

Improve peekaboo's ability to iteratively reduce error and find hidden/nonobvious features

Acknowledgements

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