Rapid IR Fuel Screening
Project 25

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Project 25

Rapid IR Fuel Screening

Stanford University

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Cost Share Partner(s): Stanford University

Objective:

Develop a **compact, low-volume prescreening tool** for the prediction of physical and chemical properties of sustainable aviation fuels (SAFs) using Fourier-Transform Infrared (FTIR) spectrometry and advanced statistical analysis methods.

Project Benefits:

- The FTIR prescreening approach will **make the SAF design and approval process less costly and more efficient**
- This low-volume (<1 mL) method yields insights that are **complementary to other prescreening approaches** (e.g., GCxGC).

Research Approach:

- Develop regularized linear and non-linear models that **correlate the physical, chemical, and combustion properties of a fuel** (e.g., boiling point, heat of combustion, flash point, etc.) **with its vapor-phase, 2-15 µm FTIR absorption spectrum**.
- Apply these models **to predict physical and chemical properties of next-generation SAFs** and fuel components.

Major Accomplishments (to date):

- **Measured spectra of 38 World Jet Fuel Survey (WJFS) samples** and **predicted molecular weights**
- Including WJFS samples in training set **improves model performance for similar fuels**
- Implemented **facility improvements** and began preliminary **measurements of liquid-phase spectra**

Future Work / Schedule:

- Begin preliminary **measurements for combined liquid- and vapor-phase training set**
- **Determine effect of phase** on the performance of property prediction models
- Develop a **combined liquid-vapor model**

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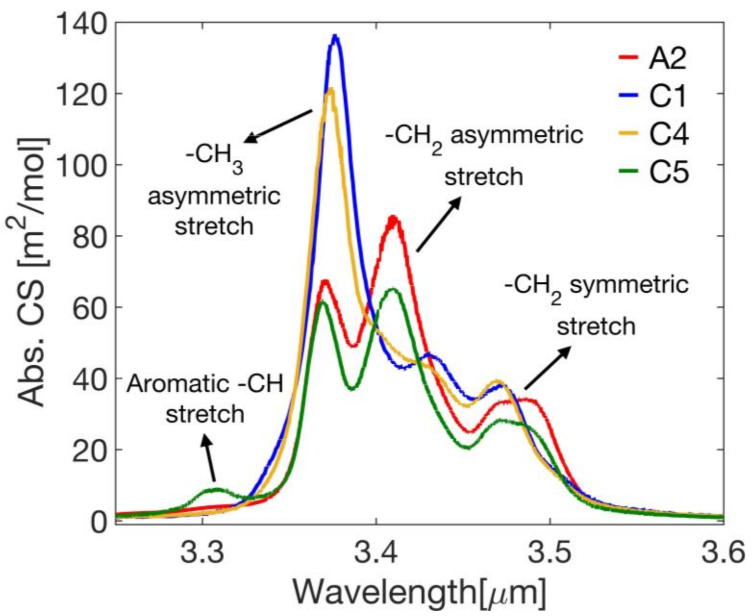
Introduction

Concept

- The vapor-phase IR absorption spectrum of a hydrocarbon fuel contains quantitative information about molecular structure and functional groups
- Statistical models can be used to infer the physical and chemical properties of fuels from this spectral information



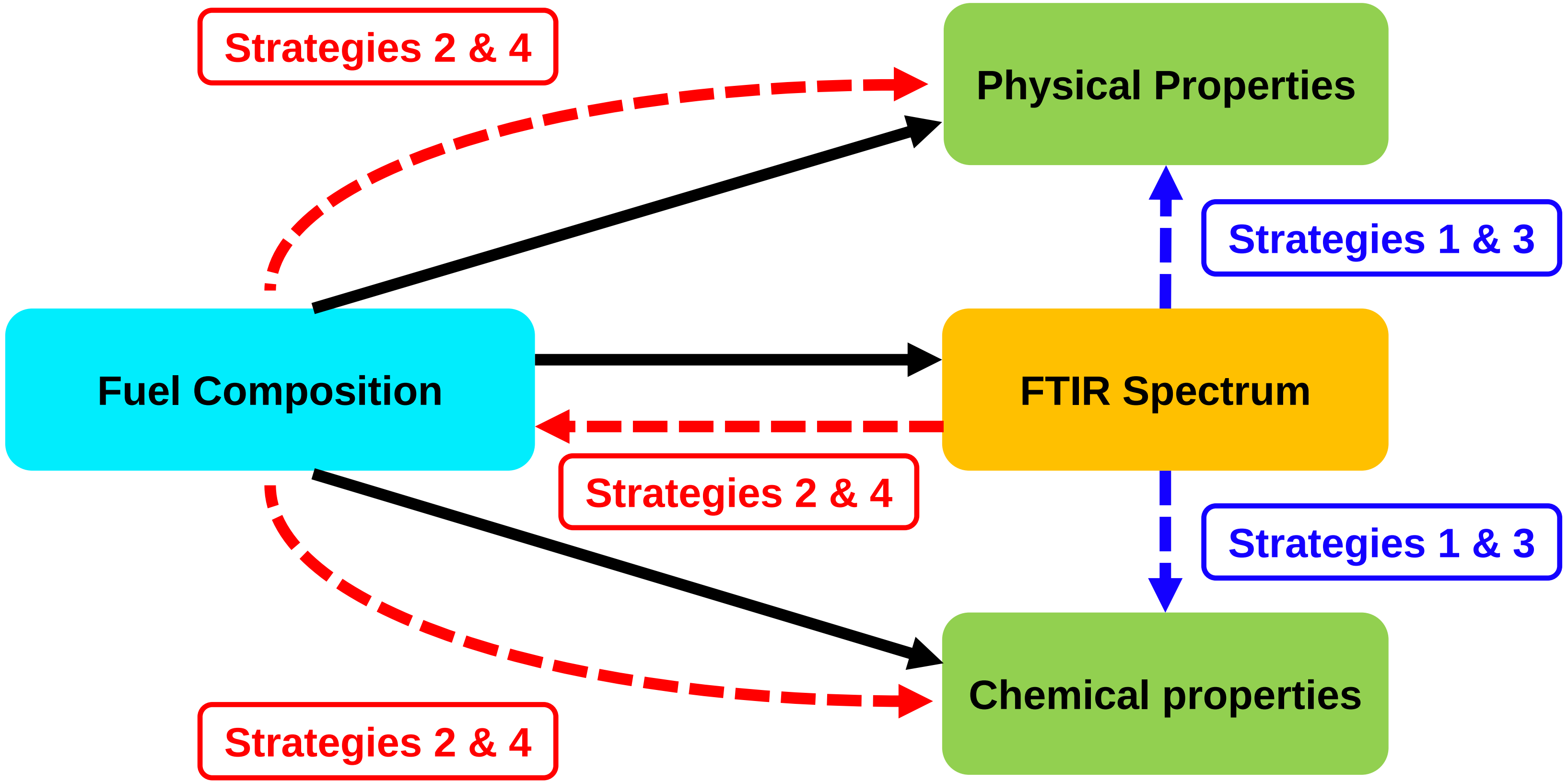
Objective

Develop a compact, low-volume prescreening tool for the prediction of physical and chemical properties of sustainable aviation fuels (SAFs) using Fourier-Transform Infrared (FTIR) spectrometry and advanced statistical analysis methods

➢ Fuel structure is evident in the IR spectra; the location and magnitude of absorption features reflect the type and number of functional groups, and can be correlated with physical/chemical properties

Broad categories of spectral analysis strategies

- Spectrum-Property Correlation Models – Strategies 1 (linear) & 3 (non-linear)
- Spectrum-Composition Models – Strategy 2 (Functional groups)
Strategy 4 (Molecular species)

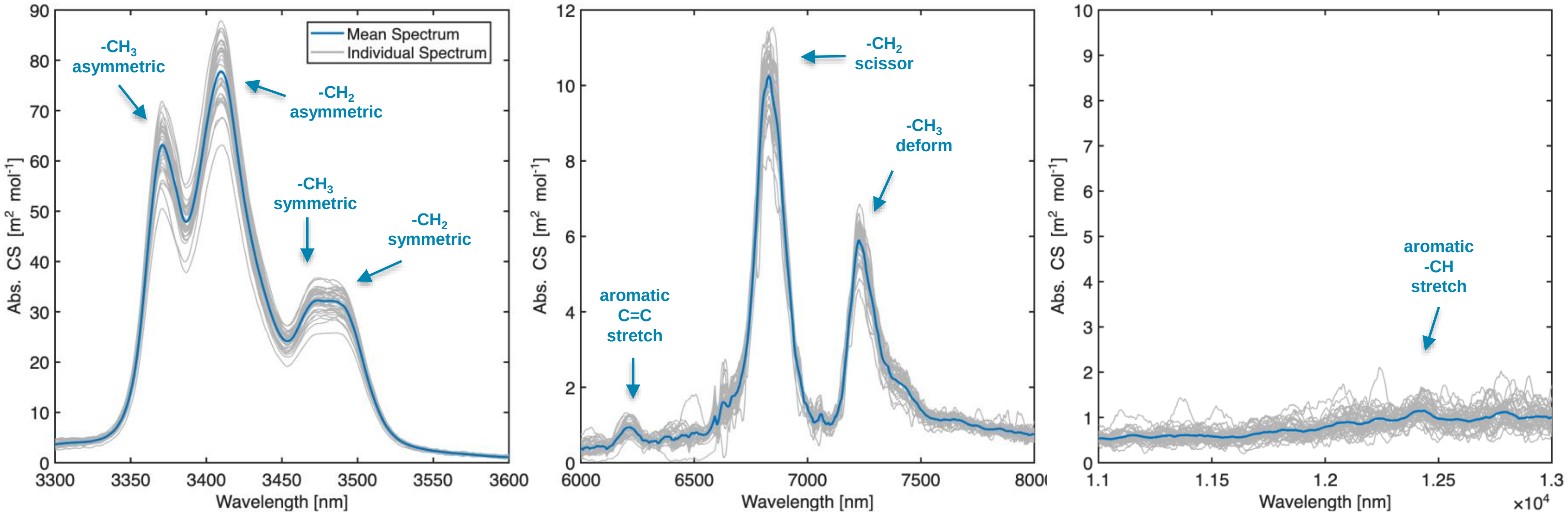


Past and Current Work

- ✓ Compared FTIR-based approaches with alternative methods in literature, revealing comparable performance
- ✓ Successfully predicted the temperature-dependent thermodynamic properties for distillate fuels
- ✓ Implemented facility improvements to allow for higher temperature and extended wavelength measurements

- ➢ ***The following slides will focus on our recent progress analyzing <u>model performance on 38 WJFS samples</u>, <u>training dataset populations</u>, and <u>preliminary comparison of vapor- and liquid-phase spectra</u>***

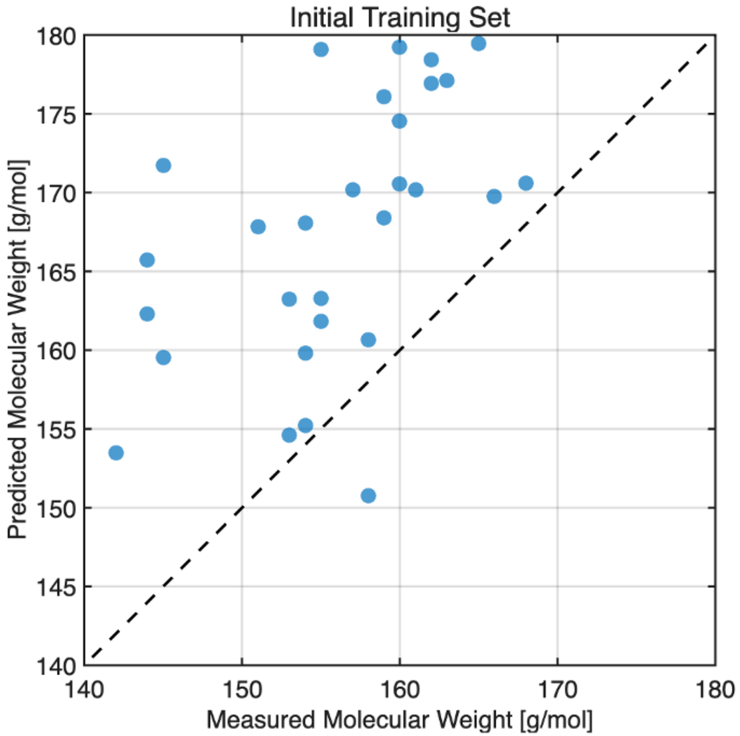
FTIR Spectra of WJFS Samples



- 38 WJFS samples were measured in the vapor-phase
- Spectral variations prominent 3 and 7 μm regions
- Differences in spectra reveal functional group and compositional variation
    - Indicates opportunity for machine learning model to relate spectral variability to property variability

First application: Prediction of molecular weight…

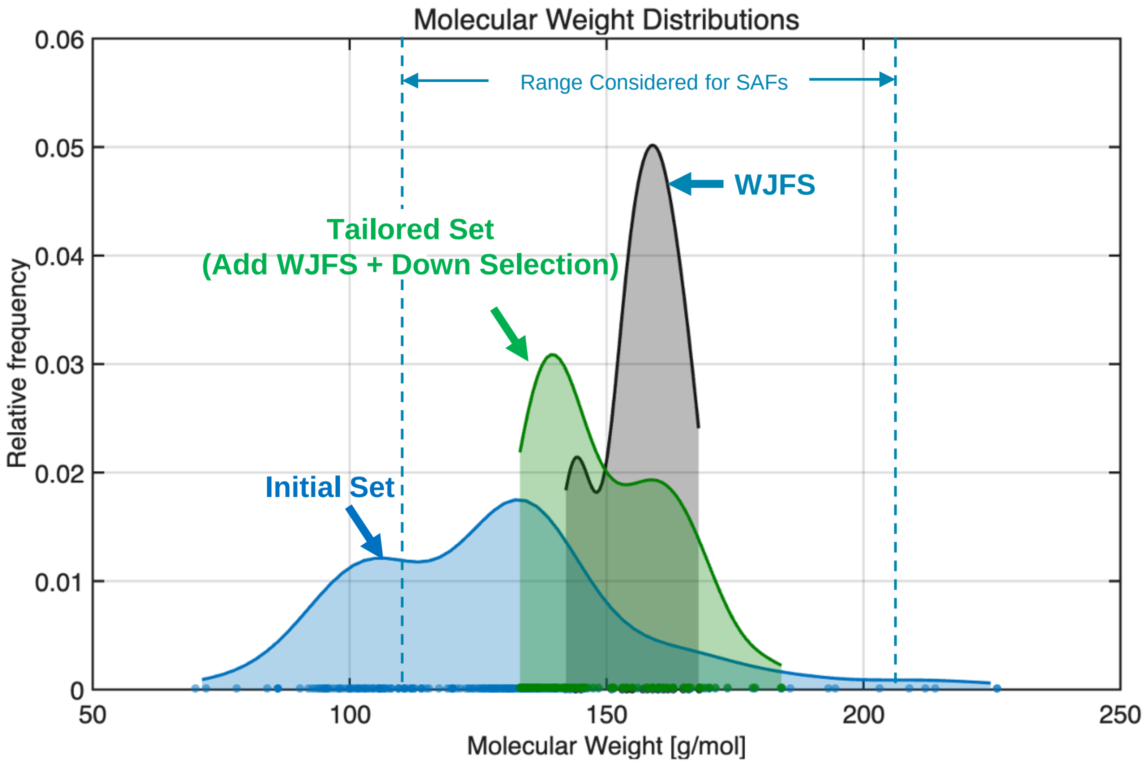
Prediction of WJFS Molecular Weights



- **Initial training set** was developed for wide range of hydrocarbons and blends, but included only 8 conventional jet fuels
- Strategy 1 was trained on this limited set and applied to the 38 WJFS samples
- Overpredicts molecular weight with a Mean Absolute Error of 15.86 g/mol
- **Why:** Training set lacks sufficient number of samples with properties closely resembling conventional jet fuel!

***Solution:** Improve training set by incorporating more conventional fuels!*

Analysis of Training Dataset Population

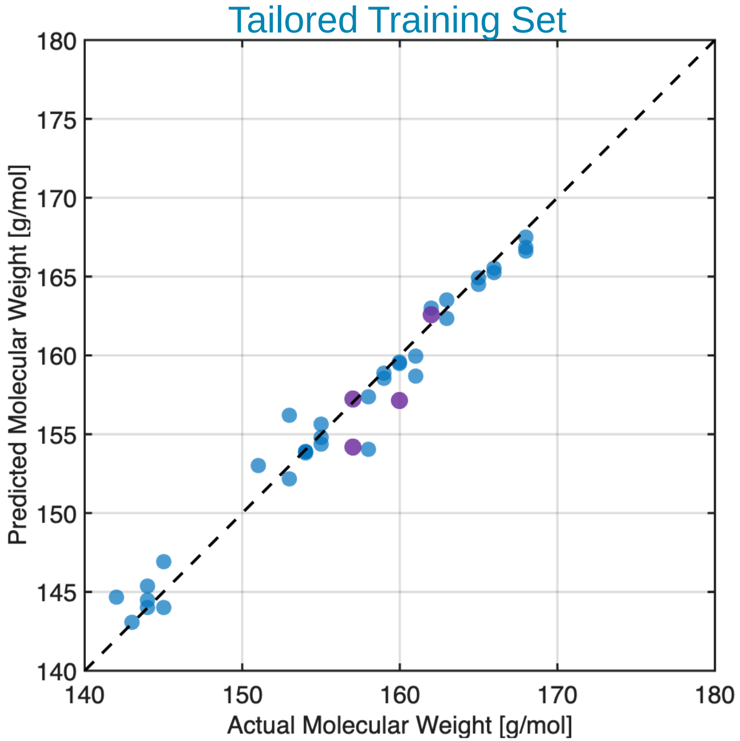


- WJFS samples show a relatively narrow distribution of molecular weight
- Initial training set spans a wider range and dips near the WJFS peak region
- Tailored set yields distribution that better represents conventional jet fuels

Emphasizes the need for a training set that reflects the target fuel types

Our broad dataset enables down-selection for tailored model development

Prediction of WJFS Molecular Weights



Size and distribution of the training set are critical for performance.

Performance improves with a larger, relevant training set.

- 34 WJFS samples were added to initial set then the total set was **down-selected to molecular weight range of 135-185 g/mol**
- This **tailored training set** better aligns with conventional fuel range while preserving a robust sample size (total of 120 spectra)
- **4 WJFS samples kept out of training process** to simulate performance on future Jet-A samples
- Tailored model yields improved predictive performance with MAE of **0.9 g/mol** for **tailored training set** and **1.6 g/mol** for the **test set**

Prediction of WJFS Molecular Weights

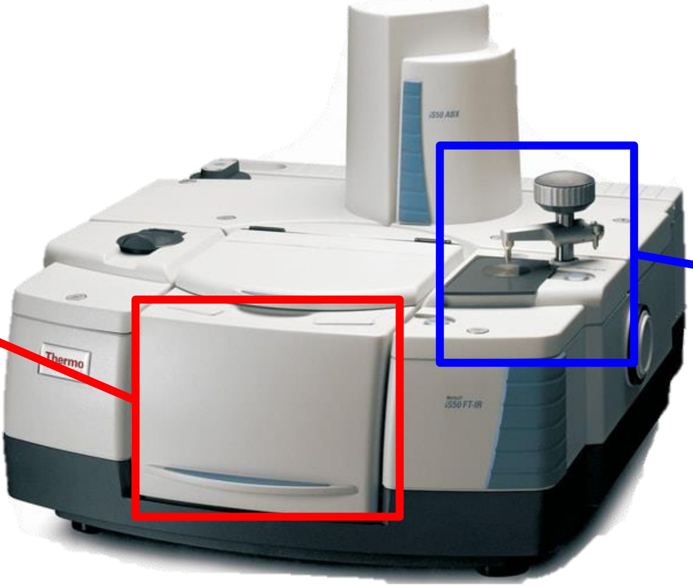
Conclusions

- Strategy 1 with limited initial training set overpredicts molecular weight of WJFS samples
- Adding WJFS samples and tailoring training set enhances model performance on conventional fuels
- Future work should expand and learn to tailor training sets for different fuel types

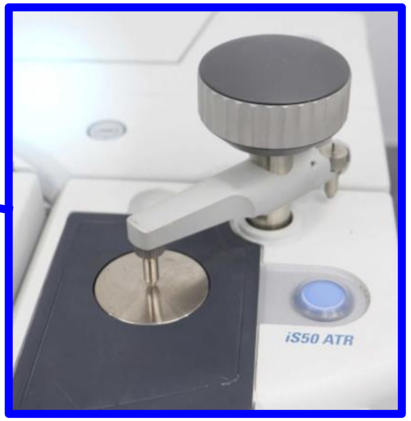
Next: Facility Improvements…

Facility Improvements

Heated Optical Cell



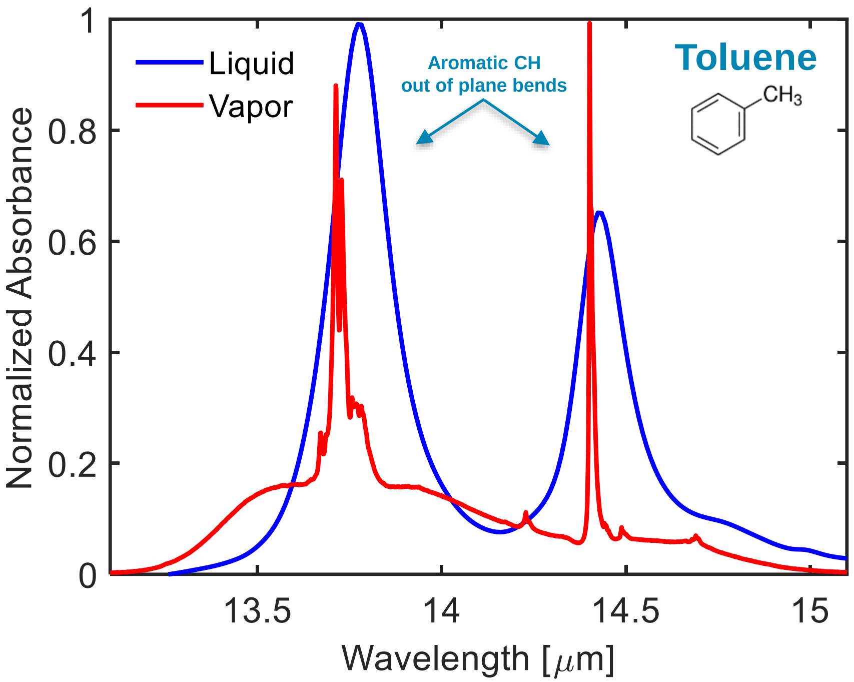
Nicolet iS50
FTIR Spectrometer



ATR Crystal

- Nicolet iS50 allows for expanded spectral range (1-200 μm), higher SNR, and better purge control and measurement of both vapor and liquid-phase
  - Heated optical cell allows for vapor-phase measurements at temperatures up to 300°C
  - ATR crystal cell used for measurement of liquid-phase samples

Comparison of Vapor and Liquid Spectra



Vapor-phase spectra

- Exhibit well-resolved fine features and follow straightforward mixing rules
- Useful for inferring composition

Liquid-phase spectra

- Exhibit broader, shifted bands
- Potentially useful for the inferring properties influenced by non-linear or intermolecular effects

Can we combine data for improved performance?

Comparison of Vapor and Liquid Spectra

Next Steps

- Compile a training set containing both vapor and liquid-phase spectra for each sample
- Determine effect of phase on the performance of property prediction models
- Develop a combined liquid-vapor model to achieve optimal performance for all properties

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- Prof. Ronald K. Hanson – Principal Investigator (rkhanson@stanford.edu)
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