Investigating Patterns Between Chemical Properties and Degradation of Per and Polyfluoroalkyl Substances (PFAS)

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INTRODUCTION

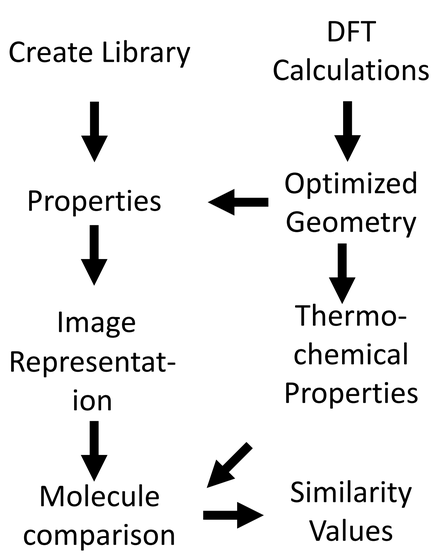
PFAS are a group of synthetic chemicals with many applications due to their water and fat repellent properties. PFAS are not easily degradable and are linked to negative health effects including cancer. Computational methods will be utilized due to difficulty gathering information experimentally. A library has been created to save and distribute information obtained and calculated on PFAS.

Thermodynamic properties will be calculated through density functional theory (DFT) at the B3LYP level with the 6-31G basis set. Key properties determined and similarities established help eliminate need to calculate properties for all PFAS.

OBJECTIVES

- Create a library containing key information for ~200 PFAS
- Calculate thermochemical properties using density functional theory (DFT)
- Identify trends and similarities within library

METHODS



RESULTS

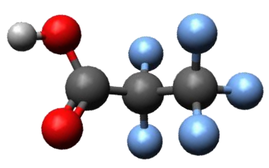


Figure 1: Perfluoropropanoic acid

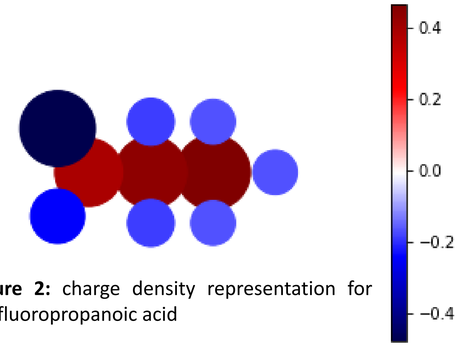


Figure 2: charge density representation for perfluoropropanoic acid

Library

Library of 193 PFAS created with use of an open-source chemistry module in Python, RDKit. Information included:

- Mass
- Van der Waals volume
- Density
- Bond information
- Atomic composition
- 2D geometries
- Charges

Images as seen in figure 2. of molecules were created using RDKit. Images represent charge density for each molecule within the library allowing for image comparison for each molecule.

The arrangement of an atom's electrons are represented in varying colors. The density of electrons within a molecule has an influence on the molecular properties of that molecule. Molecules with similar charge density return similar images and low error in image comparison.

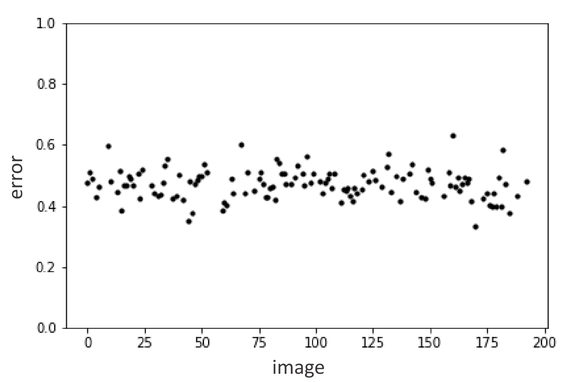


Figure 3: Perfluoropropanoic acid image comparison with 192 PFAS

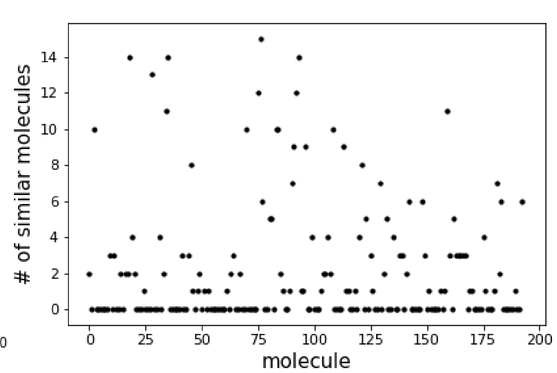


Figure 4: image comparison for 193 PFAS

CONCLUSIONS

Library

- Accessible database created containing 193 PFAS
- Comparison methods:
  - Charge density images
  - Bond and bond type similarities
  - Carbon chain length

Image Comparison

- 93 molecules with >1 similar molecules
- 100 molecules with 0 similar molecules
- Image comparison for similar molecules (e.g. PFAS w. Me, PFAS w. Et) return small difference.
- Indication of substances that ***might*** be similar

The created library will store any calculated properties, is easily shared, and amended. The function of the library to compare all PFAS contained within the library.

Future work

DFT with larger basis set will be used in future to increase accuracy of calculations. Create images with optimized geometries 2D and 3D, Natural Bond Orbital analysis. Make comparisons with different methods. Image recognition analysis developed builds foundation for incorporating machine learning into investigation.

REFERENCES

1. RDKit: Open-source cheminformatics; http://www.rdkit.org
2. Zhao, Y. H.; Abraham, M. H.; Zissimos, A. M.. J.Chem (2003)

ACKNOWLEDGEMENTS

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