Physical Chemistry

Faculty Research Interests
AY2019-2020
Overview:
We use computer models to examine thermodynamic and transport properties of alternative fuels over a broad temperature and pressure range. We can also relate the structure of the liquid fuels to the properties!

Project:

Semester 1: Simulating chemical reactions: Students learn how to write molecular dynamics computer codes for simulating the movement of atoms on computers.
Skills needed: Willingness to learn basic FORTRAN and some UNIX.

Semester 2: Computing the properties of Alternative & Surrogate Fuels
This project will develop a computer model that is capable of predicting the properties of alternative fuels of any composition even near the critical point. Compare results to experiments carried out in Chemistry Department and literature data.
Collaborators: Prof. Luning Prak & Prof. Cowart
Skills needed: Willingness to learn basic FORTRAN and some UNIX.

Past/current students: L. Herman, J. Williams, P. Lombard, R. Willingham, B. Lassen, B. Sweeney, M. Gustafson. A. C. Roa, A. Meegan

\[ \theta = 90^\circ \ (\perp) \]
\[ \theta = 0^\circ \ (\parallel) \]
We utilize spectroscopy (chiefly FT-IR) of samples at very low temperatures (10K – 140K) to examine two types of systems:

- Small stable molecules that form ices on the surfaces of comets, outer solar system bodies, or interstellar dust particles to help identify them and their irradiation products in astronomical spectra.
- Very unstable molecules, like reaction intermediates, to determine their structure, bonding and reactions

**Current Projects:**

1) **Optical Properties of Astronomical Ices:** (NASA/GSFC) - developing a spectroscopic database of the “optical constants” of simple ices (e.g. $C_2H_6$, $C_2H_4$, etc) and ice mixtures ($CH_4/N_2$, etc.) which exist in comets and outer solar system objects. May also involve ice density measurements by quartz crystal microbalance. These data are used by astronomers in modeling the composition of these objects.

2) **Raman Spectroscopy of Ices:** (USNA) testing the ability of a simple Raman spectrometer to distinguish and identify thin ice coatings on mineral samples. This will help probe the feasibility of proposed application of Raman on a Mars lander.

3) **Spectroscopy of Nitrenes and Nitrides:** (USNA) working on a unique way to make these extremely unstable intermediates, and to study them spectroscopically.

CONTACT ME FOR MORE INFORMATION!
Computational Studies of Transition Metal Systems

Overview

Potential energy surfaces of transition metal (TM) reactions
TM + CO\textsubscript{2} → Products
TM + CS\textsubscript{2} → Products

Of interest because:
- Catalysis/bond activation (C=O)
- Conversion of CO\textsubscript{2} into valuable chemicals
- Reducing CO\textsubscript{2} emissions

Previous Work (Gas phase kinetics)

TM + CO\textsubscript{2} not very reactive
TM + CS\textsubscript{2} very reactive

Objective

To understand the reactions at the molecular level by mapping the potential energy surfaces

Method

Gaussian 09 platform
Density functional theory

Required prior knowledge

SC345 - Thermodynamics & Kinetics
SC346 - Quantum Chemistry & Spectroscopy
Aim of Research: Use electroanalytical and surface science tools to accurately predict galvanic corrosion response of airframe materials in a controlled environment by performing accelerated tests on corrosion-resistant coatings (paints/primers).

Corrosion is a huge problem for Naval Aviation and the Department of Defense. One of the best ways to prevent or minimize corrosion of metals is to separate the bare metal and reactants using a coating (paint).

Many successful coatings contained Cr(VI), which has been found to be carcinogenic. The Navy is working on formulation of new anti-corrosion coatings that do not use Cr(VI).

My research uses electrochemistry and surface science to rapidly evaluate anti-corrosion properties of paints and primers, with a focus on naval aviation.

Table I

<table>
<thead>
<tr>
<th>Sample</th>
<th>1.0V</th>
<th>1.5V</th>
<th>1.8V</th>
<th>2.5V</th>
</tr>
</thead>
<tbody>
<tr>
<td>non-chromated primer on anodized Al</td>
<td>0.28</td>
<td>0.28</td>
<td>3.50</td>
<td>10.00</td>
</tr>
<tr>
<td>waterborne primer on alodine pretreated Al</td>
<td>0.25</td>
<td>0.25</td>
<td>1.60</td>
<td></td>
</tr>
<tr>
<td>chromated primer on alodine pretreated Al</td>
<td>0.28</td>
<td>0.18</td>
<td>0.18</td>
<td></td>
</tr>
</tbody>
</table>

A current project I am interested in pursuing is writing and testing a new flash photolysis kinetics experiment to study the isomerization from the cis to the trans form of o-methyl red (Larsen, M.C. & Perkins, R.J. J. Chem. Educ. 2016, 93, 2096). The project would consist of constructing the experimental apparatus, testing the procedures and writing a lab handout. It is desired that this experiment would be incorporated into the IL4 course. I am also open to other physical chemistry experiments to pursue if someone has other interesting ideas.
The following faculty are not recruiting student researchers for the 2019-2020 academic year.
OVERVIEW: My research focus is aimed at studying amyloidogenic proteins associated with neurodegenerative diseases (Alzheimer's disease, Parkinson's disease, etc.). These diseases are related to the rearrangement of specific proteins to non-native conformations. Such rearrangements promote aggregation and deposition within tissues and/or cellular compartments. Understanding the role of amyloidogenic protein interaction at solid/liquid interfaces and lipid membranes may provide valuable insight into the toxic mechanism between cellular surfaces and amyloids.

PROJECTS:

1. Measuring amyloidogenic protein interaction with lipid membranes via colorimetric assay A biomimetic, vesicle-binding assay to investigate the interactions of protein aggregates with lipid membranes. Vesicles have varied colorimetric responses when exposed to proteins depending on the extent of the protein-lipid interaction.

2. Protein aggregation and interaction affects surface chemistry Atomic force microscopy: modeling and experimentation of amyloid proteins on surfaces The aggregation and mechanical properties of surfaces and protein–lipid interactions will be studied using a various measuring techniques via AFM. Surface potential measurements and protein insertion into a lipid monolayer will be measured using a Langmuir-Blodgett trough. The potential created across the interface when amyloidogenic proteins are added provides a measure of the surface interaction of the protein.

3. Biochemical aspects of barnacle glue – NRL Collaboration. Cutting-edge biomolecular and bioinformatics approach (nanomechanics, cementomics, proteomics) to produce a comprehensive picture of the specialized proteins found in barnacle adhesives and develop underwater adhesives. Study will utilize various colorimetric/fluorimetric assay development, AFM nanomechanical studies and molecular biology to characterize proteins.

If you are interested in biochemistry, nanoscience, medical applications of chemistry, or biophysics, please see me for more information!

Past research students:
E. LaManna, M. Dorsey, C. Villareal, B. Flaherty, C. Yip, A. Schenck
Asst. Prof. Melonie Teichert
Chemistry Education

• DBER: Discipline-Based Education Research
  – Expertise in discipline (chemistry)
  – Rigorous study of teaching and learning
    (cognitive science, educational psychology,
     learning sciences)

• Research Emphasis: The Design and Assessment of Effective Learning Environments (lecture and lab)

• Projects
  – **Inquiry labs for Plebe Chemistry:** current focus is spectroscopy lab (Beer’s Law), collaboration with Monroe CC; Current Student: 1/C Diana Jacinto
  – **Guided Discovery lecture activities:** for plebe chem or upper division courses (P-Chem?)
  – **In-depth analysis of context-dependence of bond energy understanding** (plebe chem, bio, and biochem effects)
  – **Investigation of USNA faculty use of innovative teaching practices:** (Big DBER focus)
  – **Design your own project!** (Study of IL learning? Gender effects? NAPS? Let’s talk!)