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Measuring Molecular Size, Shape, and Mass with Fourier Transform Mass Spectrometry

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Areas of Interest:
Fourier transform mass spectrometry; Ion mobility; Molecular recognition; Supramolecular chemistry, especially of cucurbit[n]urils; Molecular machines
Measuring Molecular Size, Shape and Mass with Fourier Transform Mass Spectrometry

David V. Dearden
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Mass spectrometry; molecular recognition; molecular machines
FTICR/MS
Fourier transform ion cyclotron resonance mass spectrometry

Ion Cyclotron Motion

Centrifugal force: $\frac{mv^2}{r}$

Lorentz force: $qv \times B = qv_B B_z$

Cyclotron frequency: $\omega_c = \frac{2\pi}{t} = \frac{qB_z}{m}$
Advantages of FTICR/MS

- Ultra-high mass resolving power
  - $m/\Delta m > 10^6$
- Accurate mass measurement
  - To about 1 ppm over a wide mass range
- Allows determination of molecular formulas
- Ion storage and manipulation
  - Contents of the trap are easily controlled
    - Reaction studies
    - Complicated mixtures
    - Structural information through $MS^n$
    - Prolonged irradiation
A New Way to Measure Molecular Size

\[ y = a + bx \]
Coefficient values ± one standard deviation
\[ a = 63.858 \pm 2.11 \]
\[ b = 0.6205 \pm 0.0155 \]
\[ R^2 = 0.988 \]
A New Way to Measure High Vacuum
Polymer-Nanoparticle Composites for Catalysis, Conducting Polymers, and Light Harvesting Technologies

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Chemistry and Biochemistry
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Areas of Interest:
Organic Synthesis; Catalysis; Materials Science; Nanoparticle catalysis; Inorganic Synthesis; Biocatalysis
Polymer-Nanoparticle Composites for Catalysis, Conducting Polymers, and Light Harvesting Technologies

David Michaelis
Department of Chemistry and Biochemistry
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Traditional polymer supports                      Dual optimization approach

modify nanoparticle composition  tune metal–support interaction

metal–support interaction

Polymer-supported heterobimetallic nanoparticle catalyst

RuCl₃·H₂O + M₂  poly(styrene) (25000 MW) NaBH₄
EtOH  no processing required

commercially available polymer support

2% Ru-P.S. NH₂NH₂·H₂O (3 equiv)
EtOH, r.t.

% conversion

time (minutes)

Ph
0  20  40  60  80  100
0  100

2% Ru–P.S.
NH₂NH₂·H₂O (3 equiv)
EtOH, r.t.

2

1

2a

2a

1a

97% 94% 93% 98% 99%
10 h 10 h 8 h 5 h 4 h

6a X = H
6b X = CF₃
6c X = Me
6d X = OMe
Heterogeneous Catalysis, Conversion of Biofuels and CO₂

Kara Stowers
Chemistry and Biochemistry
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(801) 422-0835

Areas of Interest:
Metal catalyst synthesis and characterization, Organic transformations, Mechanistic studies, Heterogeneous phase catalysis
Heterogeneous Catalysis, Conversion of Biofuels and CO$_2$

Kara Stowers
C405 BNSN
422-0835
Inorganic synthesis of Heterogeneous Catalysts

- CO\(_2\) is typically kinetically unreactive but metal catalysts can react with CO\(_2\).
- Separation is good with heterogeneous catalysts.
- Bimetallic alloys, supported/unsupported nanoparticle metals

**Potential Collaboration:**
Catalyst surface modeling
Gas-phase Reactivity of CO₂

- CO₂ and hydrocarbons will be used as reagents.
- Many possible reagents for reactivity (alkenes, alkynes, chlorinated reagents, epoxides).

Potential Collaboration:
Atypical reactions with difficult selectivity outcomes
Mechanistic Studies on Catalyst Surfaces

- Spectroscopy allows *in situ* characterization of catalysts and info about active sites.
- Temperature programmed reaction can determine mechanism, activation, and deactivation.

Potential Collaboration: TPRS, *in-situ* analysis
Mechanism of Assembly of Cell Signaling Complexes

Barry M. Willardson
Chemistry and Biochemistry
bmwillardson@chem.byu.edu
(801) 422-2785

Areas of Interest:
Cell signaling; Chaperone-mediated assembly of signaling complexes; Neurodegenerative diseases
Mechanism of Assembly of Cell Signaling Complexes

Barry M. Willardson
Department of Chemistry and Biochemistry
G protein Signaling Cycle

Mechanism of G protein complex assembly

Nascent Gβ + CCT → PhLP1-Gβ → PhLP1-Gβγ → G protein heterotrimer
Structural analysis of the Gβ-CCT complex
Structural analysis of the PhLP1-Gβ-CCT complex

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<td>280</td>
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<th>Lys 2</th>
<th>Dist (Å)</th>
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Security

Kent Seamons
Computer Science
Internet Security Research Lab
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Areas of Interest:
Easy secure data sharing; Privacy; Digital credentials and trust negotiation
Security

Research Interests
- Easy secure data sharing
- Privacy

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Easy Secure Data Sharing

- Problem: no end-to-end encryption
  - Google can read your email
  - Government surveillance
  - Hackers
- Encryption solutions are too hard to use
Secure Webmail

- BYU design and prototype
- User studies show problems with:
  - Trust
  - Understanding
  - Occasional mistakes
Potential Collaborations

• Human experts, Statisticians
  • How to measure human understanding and trust
  • Help with survey questions
  • New measurement methods geared for security
  • NSF funding targeted for interdisciplinary teams of computer security experts along with behavioral and social scientists
Privacy

you

https://mail.google.com/

facebook

GOOD GOOD
2.8 million tests in 2 weeks

12,000 MITM detections
<table>
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<th>Proxy Type</th>
<th>Connections</th>
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<td>Personal Firewall</td>
<td>6,384</td>
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<tr>
<td>Enterprise Firewall</td>
<td>463</td>
<td>3.94%</td>
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<tr>
<td>Personal/Enterprise Firewall</td>
<td>1,528</td>
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<td>Organization</td>
<td>1,448</td>
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<td>Malware</td>
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<td>Unknown</td>
<td>880</td>
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Potential Collaborations

- Human experts, Statisticians
  - How to better measure user attitudes toward surveillance
  - Design user interface for notice and consent
  - Design user studies to measure effectiveness
- Math/crypto experts
  - Next-generation trust model that goes beyond certificates
Computational Creativity: Machines as Colleagues

Dan Ventura
Computer Science
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(801) 422-9075

Areas of Interest:
Neural networks; Applied Machine learning; Artificial intelligence; Evolutionary computation; Computational creativity
Computational Creativity: Machines as colleagues

Dan Ventura
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Applied Machine Learning

- Features
- Data
- Model Class

Learning Algorithm

Model

- classification
- control
- inference
- imputation
- identification
Computational Creativity

The philosophy, science and engineering of computational systems which, by taking on particular responsibilities, exhibit behaviours that unbiased observers would deem to be creative.

Colton & Wiggins

Invention  Ideation  Learning

Skill  Appreciation  Imagination

Reflection  Intentionality  Accountability
The arts

Cooking

**Recipe 1: Scrumptious Broth with Bean**

**Ingredients:**
- 2 3/8 cups - vegetable broth
- 2 1/3 cups - chicken broth
- 1 1/3 cups - coconut milk
- 1 cup - halloumi
- 1 cup - leek
- 2 1/2 sticks - cinnamon
- 7/8 cup - yellow onion
- 1 1/2 green chile
- 3 5/8 tablespoons - lemon juice
- 1/4 cup - white onion
- 1/4 cup - crushed tomato
- 1/2 red bell pepper
- 1/8 cup - green onion
- 1/8 cup - vegetable juice
- 1 5/8 tablespoons - green tea
- 1 1/2 tablespoons - asiago
- 1 3/8 tablespoons - sherry
- 1/8 cup - black beans, precooked
- 1 tablespoon - evaporated milk
- 1 3/8 teaspoons - baking cocoa
- 1 1/3 teaspoons - pepper

**Directions:** Combine ingredients and bring to boil. Reduce heat and simmer until done, stirring occasionally. Serve piping hot and enjoy.

Music

Visual Art
What about the sciences?
Questions:

- In what ways does the domain I work in require creativity?
- Does it make sense to think about automating some of that creativity?
Leadership in Mentoring

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Mathematics
deniseh@math.byu.edu
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Areas of Interest:
Mentoring leadership; Student mentorship; Geometric Topology; Geometric Optimization; Mathematics of Origami and Design
Leadership in Mentoring

by Denise Halverson

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Leadership

Leadership is doing what is right, valuing others as children of our Heavenly Father, and pursuing the greatest good for all by applying correct principles.

“Management is doing things right; leadership is doing the right things.”

~Warren Bennis

“My definition of leadership is communicating to people their worth and potential so clearly that they are inspired to see it in themselves.”

~Stephen R. Covey
MathFest 2013, Hartford, CT
Why Implement Leadership Practices in Mentoring?

- Students feel empowered as life long learners.
- Students develop their own personal mission statements.
- Students learn and implement universal principles in their lives:
  - Continuous learning
  - Service
  - Positive energy
  - Viewing others as children of our Heavenly Father
  - Balance
  - Excitement for life and its opportunities
  - Self-renewal
- Students are enabled to stand up and speak up for what is right, what really works, and the good of all.
Teaching and Leadership Presentations

Fall 2014 Schedule

Monday, September 15th

Leadership Foundations – John Bingham
ESC C-295, 4-5 pm

Monday, October 13th

Global Leadership - Gregg Warnick

Monday, November 10th

Reaching Out - Kent Crookston