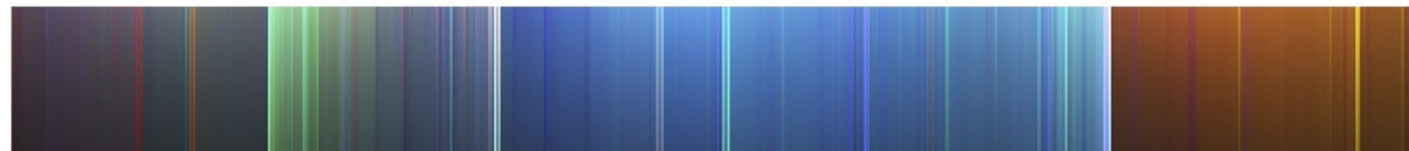


# NSF/CHE Virtual Office Hour

## Hispanic Heritage Month Celebration

October 16, 2020

(Please mute your mics; Submit questions through the chat feature.)



# Featured Panelists



Dr. Héctor Abruña  
Cornell University



Dr. Carlos Baiz  
U Texas, Austin



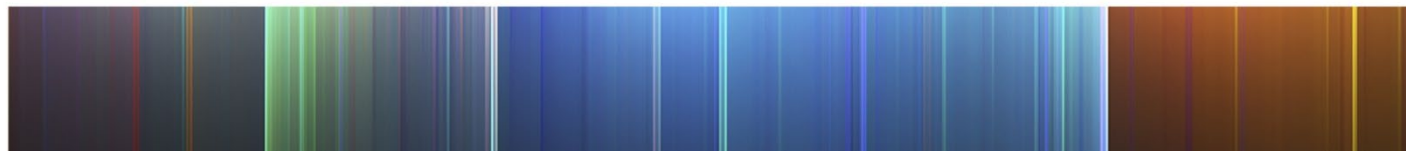
Dr. Daniel Romo  
Baylor University



Dr. Daniela Kohen  
Carleton College



Dr. Maria Oliver-Hoyo  
NC State University





## Héctor D. Abruña



### *Personal Information:*

Born: November 8, 1953 in San Juan, Puerto Rico; US Citizen.

### *Education:*

B.S., Chemistry 1975 M.S. Chemistry 1976 Rensselaer Polytechnic Institute

Ph.D. 1980 (Electrochemistry) University of North Carolina, Chapel Hill

(R. W. Murray, T. J. Meyer advisors)

Post-Doc: 1980-81 Univ. of Texas at Austin (A. J. Bard advisor)

### *Selected Professional Experience:*

August 1, 2018 -

Director, Center for Alkaline-Based Energy Solutions (CABES)

July 1, 2004 – June 30, 2008

Chair, Department of Chemistry, Cornell University

1994 – Present

Emile M. Chamot Professor, Dept. of Chem. Cornell Univ.

1991 – 1994

Professor, Dept. of Chem. Cornell Univ.

1988 – 1991

Associate Professor, Dept. of Chem. Cornell Univ.

1983 – 1988

Assistant Professor, Dept. of Chem. Cornell Univ.

1982 – 1983

Assistant Professor Dept. of Chem. Univ. of Puerto Rico

### *Selected Recent Awards:*

ACS Award in Analytical Chemistry, American Chemical Society, 2021

Award for Experimental Electrochemistry, International Society of Electrochemistry, 2021 Frumkin

Medal, International Society of Electrochemistry 2019

Allen J. Bard Award in Electrochemical Science, 2019

Elected Member of the National Academy of Sciences, 2018

Gold Medal International Society of Electrochemistry 2017





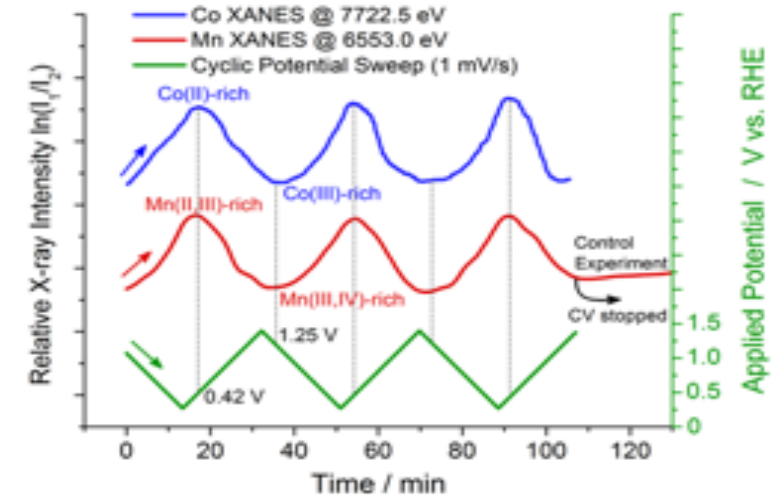
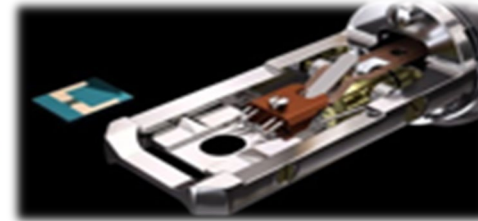
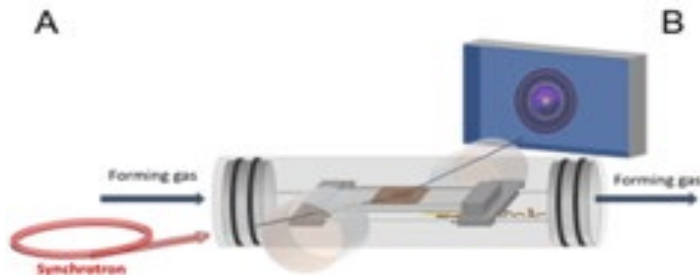
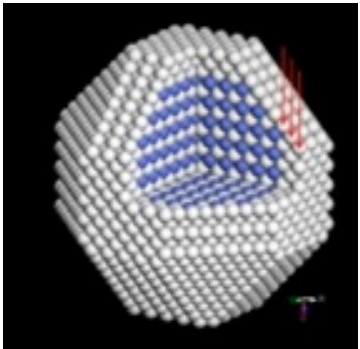
# Electrochemistry

- Electrocatalysis and fuel cells

- ❖ Use of ordered intermetallics as electrocatalysts

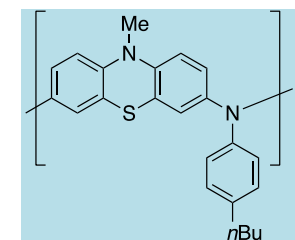
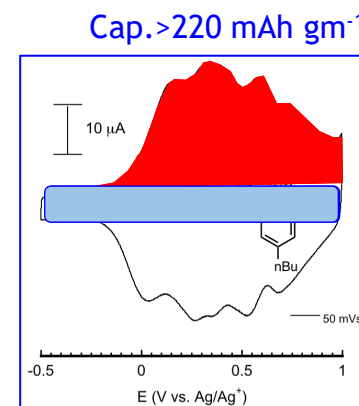
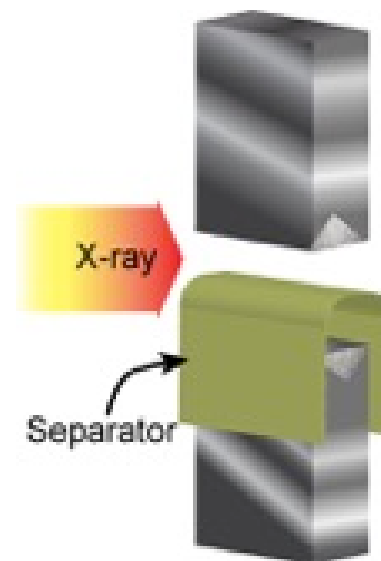
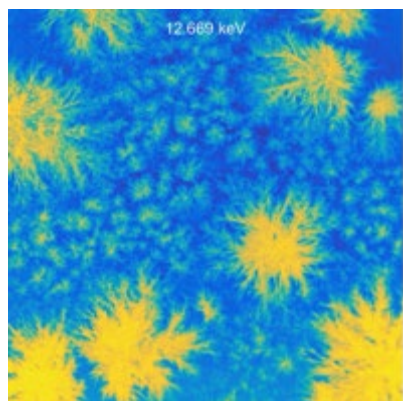
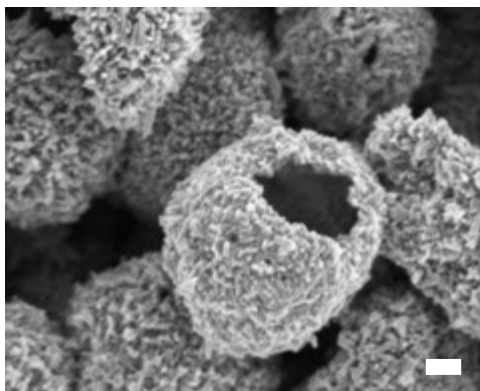
- ❖ Quantitative Studies of Disorder-Order Phase Transition in  $\text{Pt}_3\text{Co}$

- ❖ MnCo Oxide Spinel for ORR in Alkaline Media



# Electrochemistry

- Batteries & Supercapacitors:
  - ❖ Li/S and Li/Se batteries
  - ❖ Li metal deposition
  - ❖ New organic cathode materials
  - ❖ RAS-CP composites as supercaps



## Professional Accomplishments:

Abruña is an internationally recognized leader in electrochemistry and analytical chemistry with 515 publications (h-index of 92). His contributions are both deeply fundamental and technologically relevant. His thesis research was part of the genesis of chemically modified electrodes.

At Cornell, he pioneered the application of X-ray methods to the *in-situ* study of electrochemical interfaces especially the underpotential deposition of metal monolayers on single crystal surfaces. He pioneered the development of redox and photoactive nanometric molecular building blocks for the modification of electrode surfaces for applications in (bio)sensors, catalysis and LEDs. He and colleagues in Physics provided the first example of a single-molecule transistor exhibiting Coulomb Blockade and Kondo resonance. Abruña and DiSalvo demonstrated that ordered intermetallic phases such as PtBi and PtPb can exhibit extraordinary electrocatalytic activity for fuel cell

applications. He developed high performance electrocatalysts for the oxygen reduction reaction (ORR) based on core/shell structures with ordered intermetallic cores and metallic shells. Abruña and Muller pioneered the application of TEM to the in-situ study of fuel cell electrocatalysts and lithium ion battery materials.

Abruña has made major advances in the application of DEMS (differential electrochemical mass spectrometry) to the study of reaction mechanisms of relevance to fuel cells as well as degradation pathways for lithium ion batteries and carried fundamental studies of organic materials for batteries and graphene as an electrochemical platform.

An integral part of Abruña's professional accomplishments derives from his deep commitment to education and minorities. He considers his 56 Ph.D. students and 70 Post-Doctoral associates as his most important professional achievement.





JOURNAL OF  
**CHEMICAL EDUCATION**

### Energy in the Age of Sustainability

• Hidir D. Abnur\*

\* Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853-5501, United States



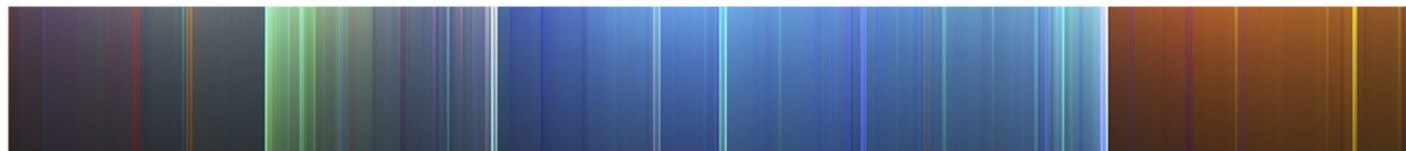




## Carlos Baiz

Assistant Professor  
Department of Chemistry,  
University of Texas at Austin

Carlos Baiz is a faculty member at the University of Texas at Austin. His group studies the biophysics of complex systems such as heterogeneous lipid membranes and membrane proteins using ultrafast two-dimensional infrared spectroscopy and molecular dynamics simulations. He has a Ph.D. in Chemistry from the University of Michigan where he worked in the lab of Prof. Kevin Kubarych and postdoctoral training at MIT and University of Chicago with Prof. Andrei Tokmakoff.

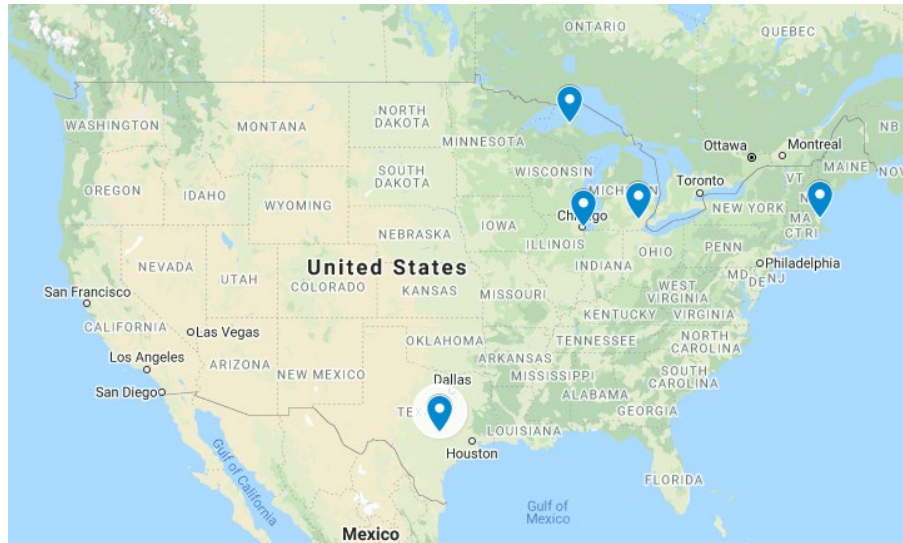


# CARLOS BAIZ (Brief Bio)

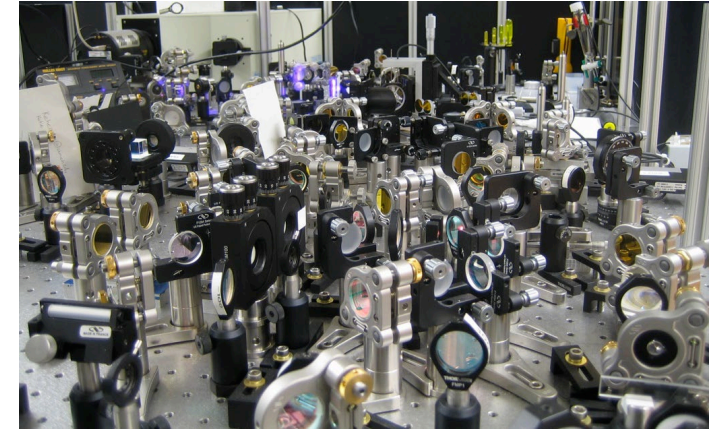
Originally from Uruguay



B.S: Michigan Tech Univ.  
Ph.D: University of Michigan  
Postdoc: MIT and UChicago.

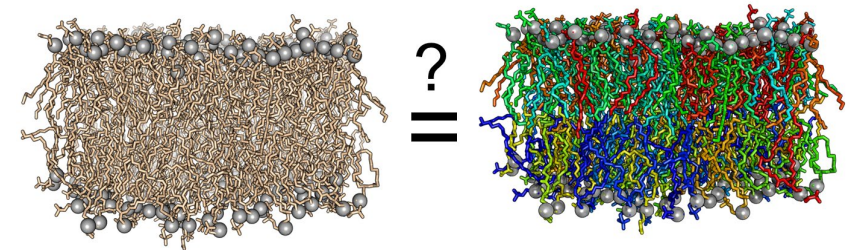


Training in ultrafast spectroscopy  
and molecular dynamics simulations



Research Areas:

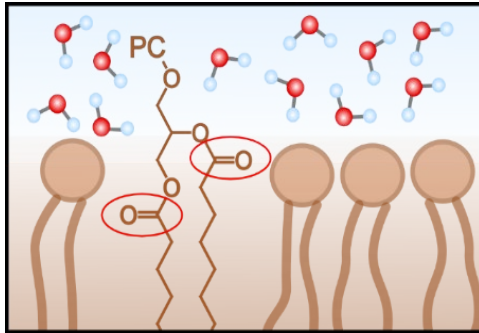
- Biophysical Chemistry
- Ultrafast methods development
- Modeling and simulation of IR spectra



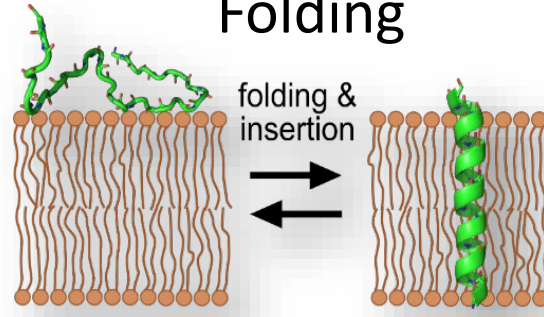


# BAIZ GROUP RESEARCH OVERVIEW

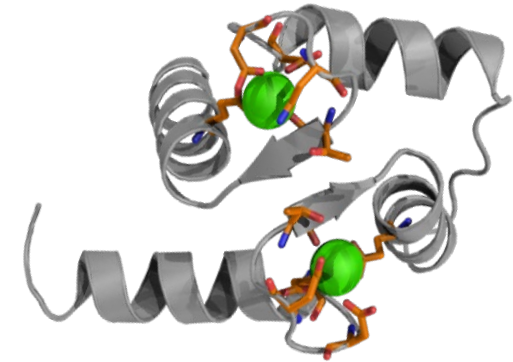
## Membrane Interfaces



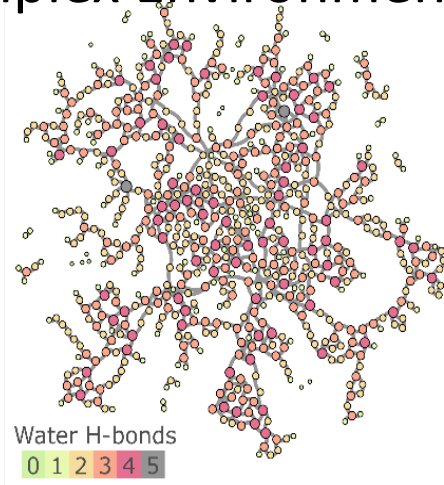
## Membrane Protein Folding



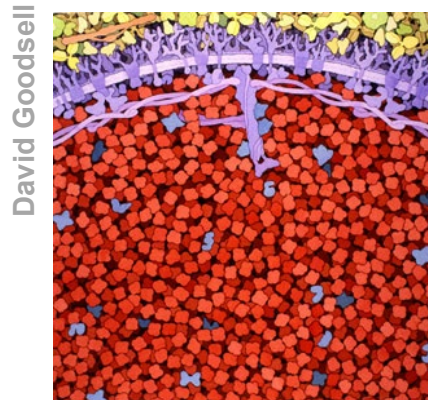
## Ion binding



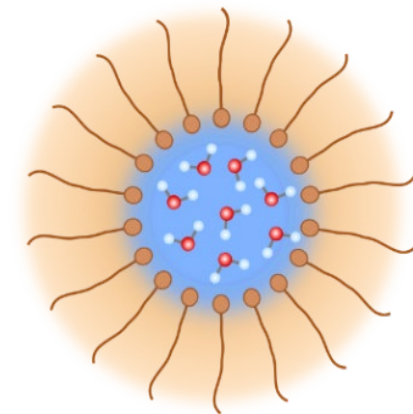
## Complex Environments



## Confined water



## Surfactant Interfaces



# GRADUATE RECRUITING PROGRAM (NSF Broader Impacts)

Student Preview of University Research and Scholarship (SPURS)



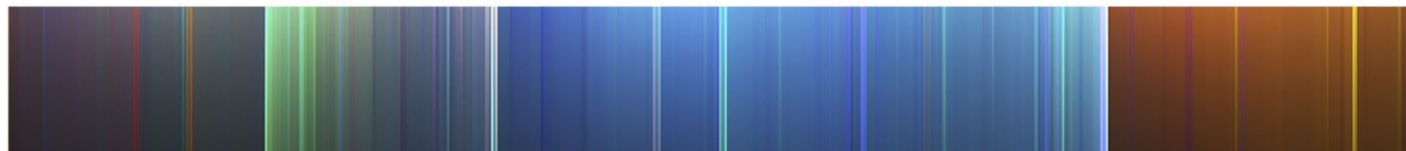




## Daniel Romo

Schotts Professor of Chemistry  
Dept. of Chemistry & Biochemistry  
Baylor University

*Romo Group research interests are at the interface of chemistry and biology focused on application of pharmacophore-directed retrosynthesis toward mechanism of action studies of bioactive natural products. Synthetic methodology focused on new organocascade processes including those directed toward the synthesis of  $\beta$ -lactones and their application as intermediates for organic synthesis and utility as proteomics probes.*



**San Antonio, West Side to NW side  
“Moving on Up”**

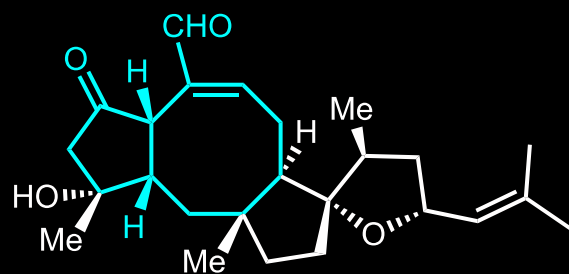
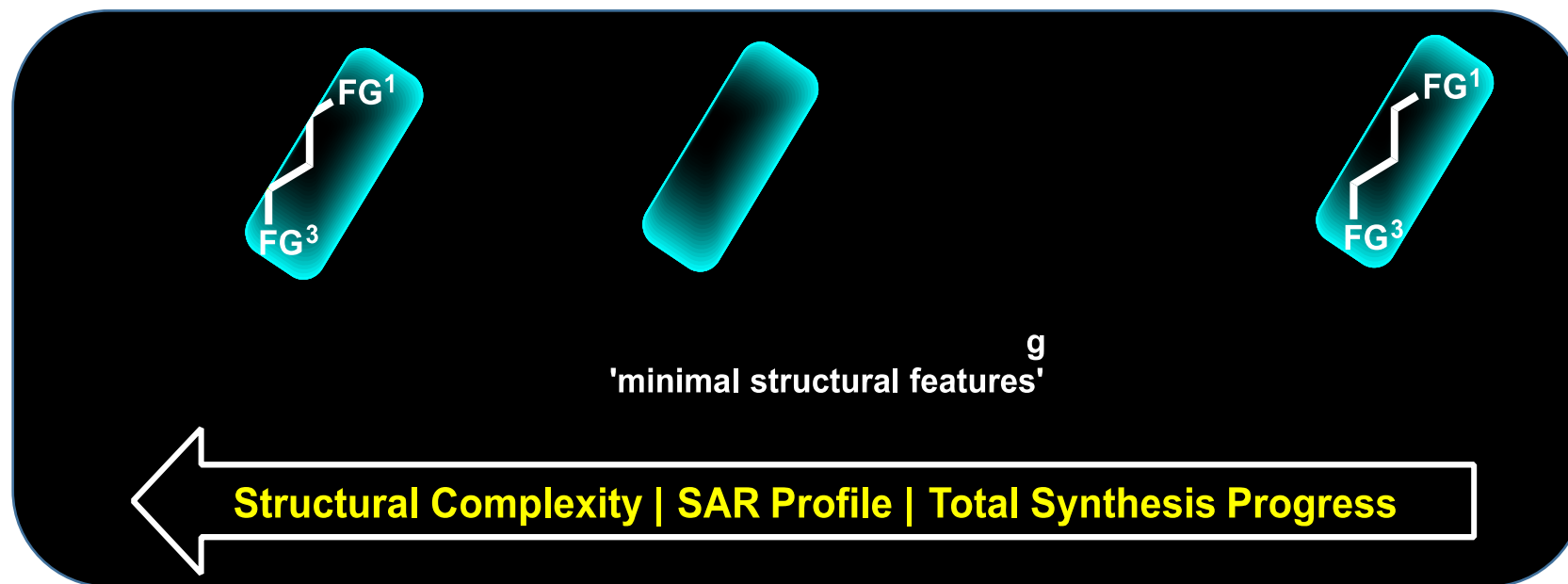
**2<sup>nd</sup> Generation Mexican-American  
-Pancho Villa**

**Cotton Pickin’ Grandfather (‘granpo’)-1920’s**



**TAMU: 1993-2015  
Baylor: 2015-**

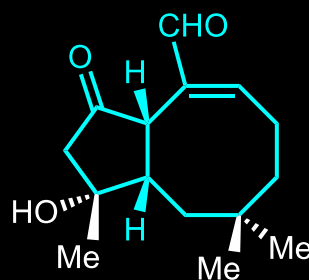
# Pharmacophore-Directed Retrosynthesis: Marrying Total Synthesis & Structure-Activity Relationships



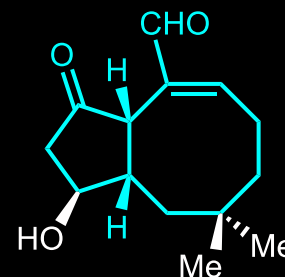
**(-)-ophiobolin A**

**MDA-MB-231**  
(ED<sub>50</sub>,  $\mu$ M)

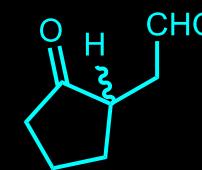
**0.61**



**11.9**



**9.5**



**>60**

Structural Complexity | Total Synthesis Progress | SAR Profile



## Daniela Kohen Chemistry Professor Carleton College

Daniela Kohen is an Argentinian Physical Chemist that teaches at Carleton College, a very small and highly selective liberal art college in Minnesota.

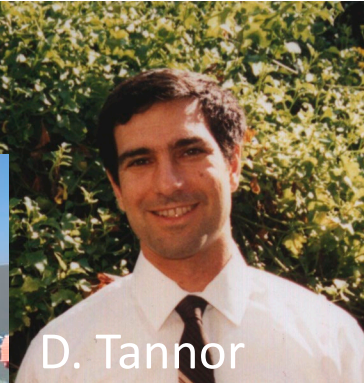


# PHASE SPACE DISTRIBUTION FUNCTION APPROACH TO MOLECULAR DYNAMICS IN SOLUTION

A Dissertation



UNIVERSITY OF  
NOTRE DAME



D. Tannor



C. Martens

UCI

University of  
California, Irvine



SMITH  
COLLEGE



Lucent Technologies  
Bell Labs Innovations



Bell Laboratories



F.  
Stillinger

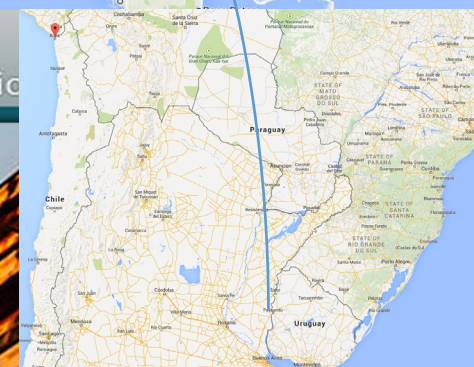


J. Tully

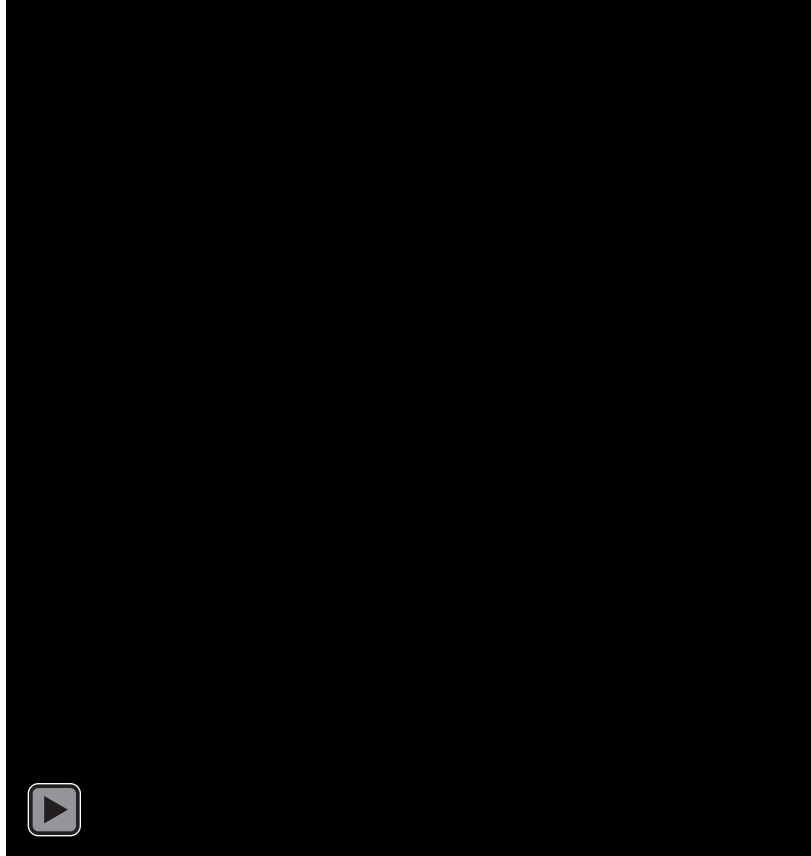


Facultad de Ciencias Exactas y Naturales  
UBA EXACTAS

Institución

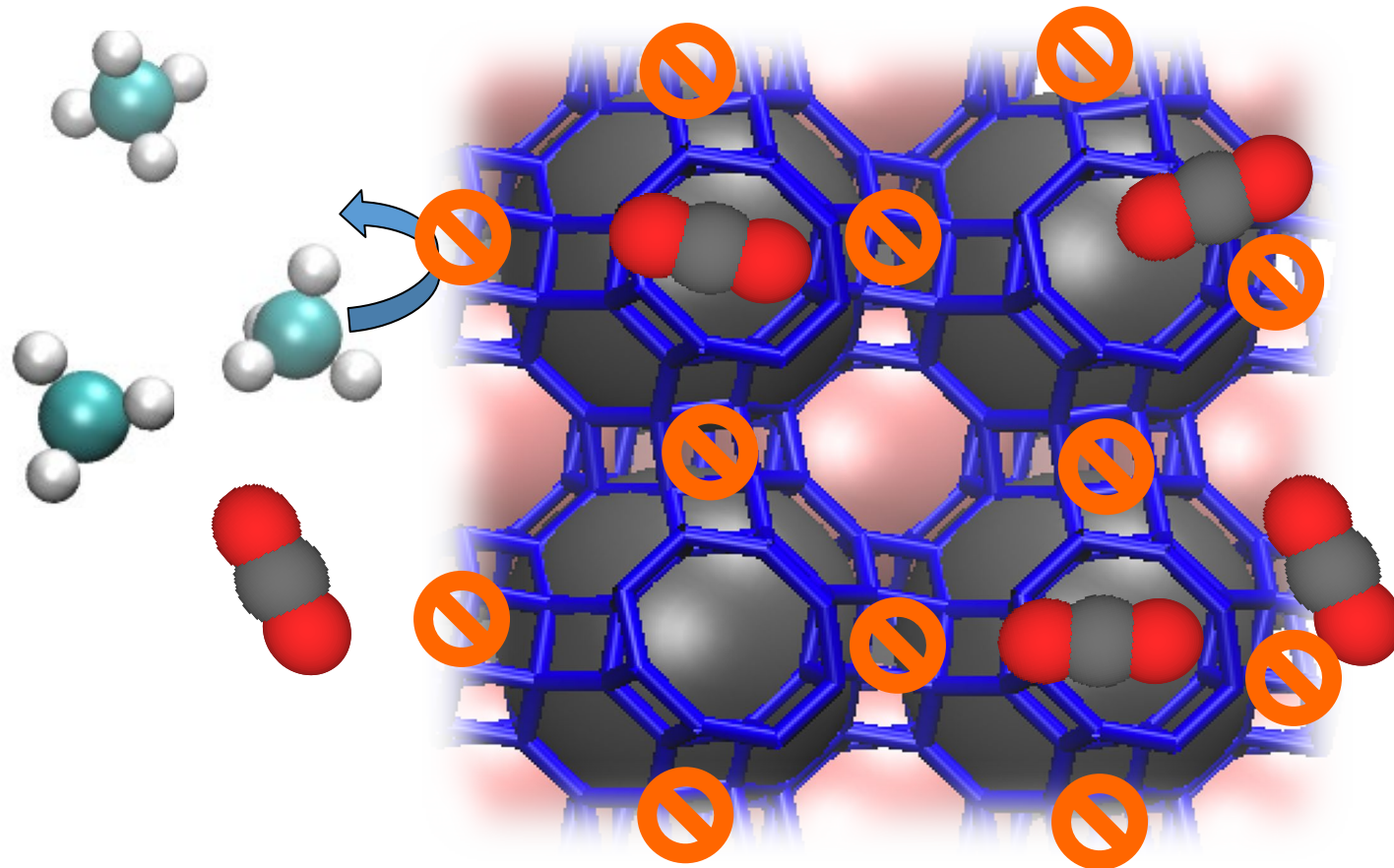


# Using Computational Chemistry to Study Motion within Zeolites





# Molecular Insight into CO<sub>2</sub> “Trapdoor” adsorption within zeolite Na-RHO

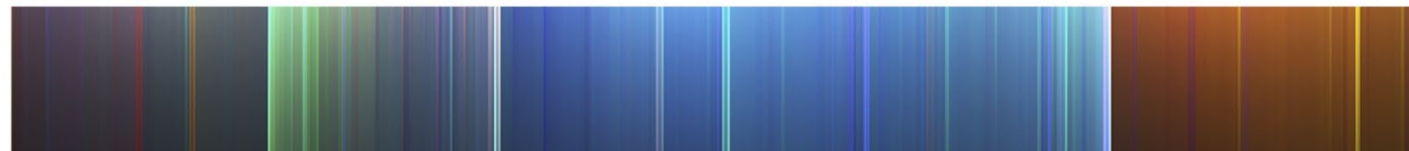


Carbon Dioxide strong interactions with apertures allows it to squeeze by “swinging” cations



*Maria Oliver-Hoyo*  
*North Carolina State University, Raleigh, NC*  
*Associate Dean for Academic Affairs, College of Sciences*  
*Professor of Chemistry*

Tenured career at NC State since 1999 moving  
into administration in July 2019.





# *Personal/career story*



# *Research Interests*



## Chemistry Education Research (CER)

- Challenges: intersection of science and education  
: three realms in chemistry
- Theme: visualization of chemical phenomena  
: visualization in tangible and cognitive ways (i.e. representational competence)
- NSF connections: CAREER award 2004  
: EHR/DRL rotation 2012-2014