Miliordos computational chemistry research group

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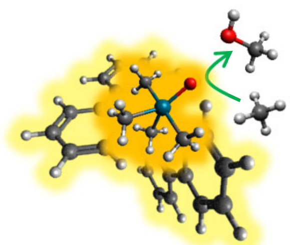
Auburn, 8/24/2024

Miliordos group: Computational Catalysis and Materials with Diffuse Electrons

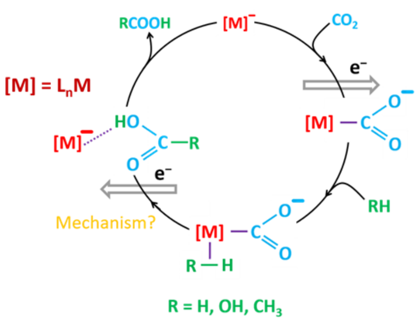
Computational Catalysis

What is the optimal combination of metal and ligands?

Converting methane to methanol selectively using molecular catalysts



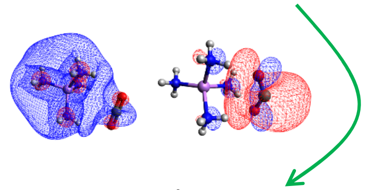
Capture and utilization of CO_2 using transition metal anionic centers



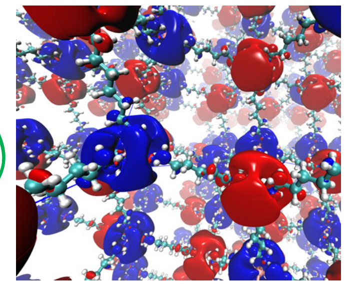
Chemistry of diffuse electrons

Capturing, reducing and valorizing CO_2

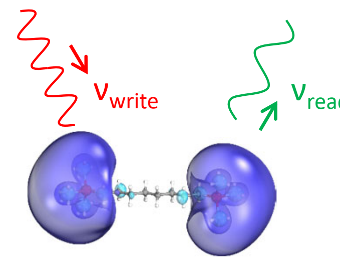
$CO_2 + H_2C{=}CH_2$



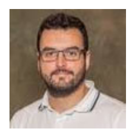
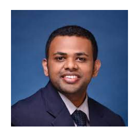
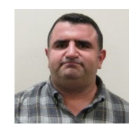
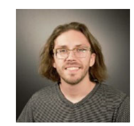
Lactones, polymers



Quantum computing

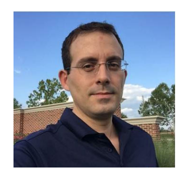


Former members

OEHHA California Office of Environmental Health Hazard Assessment | LANL | GT | ND | PNNL | Michigan State

More info / current members / publications



https://aub.ie/miligroup

Email: emiliord@auburn.edu

Products and Collaborations

More than 60 articles over the past seven years (3 highlighted, 10 invited):

Physical Chemistry Chemical Physics; Journal of Physical Chemistry A; Journal of Physical Chemistry C
Journal of Chemical Physics; Journal of Computational Chemistry; Computational and Theoretical Chemistry
International Journal of Quantum Chemistry

Angewandte Chemie; Chemical Communications; Journal of Physical Chemistry Letters; Science

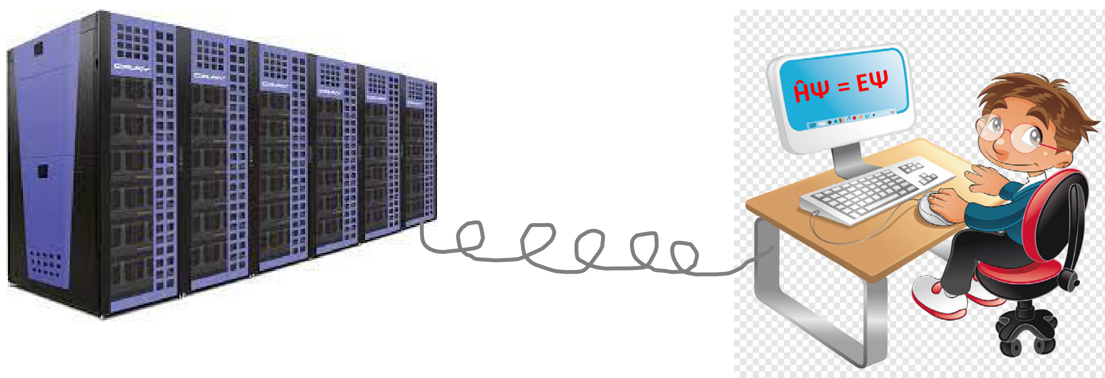
Journal of Chemical Education; Inorganic Chemistry; Journal of Quantitative Spectroscopy and Radiative Transfer

10 Journal covers:

PI: 20 invited and 7 contributed talks
Students and post-docs: 25 posters and 10 talks

We are a computational chemistry group

We solve the Schrödinger equation for molecular systems with the use of supercomputers and collaborate with experimentalists to assist them or confirm our findings



Fascinating part: We describe nature / predict phenomena with no information except for $\hbar$, m_e, m_p, q_e

AU Collaborators: J. V. O. Ortiz, F. L. Pawłowski, K. J. Patkowski, J. Harshman, C. Glodsmith, A. Adamczyk
External Collaborators: K. H. Bowen (JHU), A. Gorden (Texas Tech), M. A. Duncan (UGA), R. Signorell (ETH-Zurich), K. Vogiatzis (UTK)

Our interests

1) **Design of new materials with diffuse electrons**

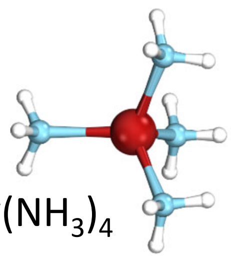
   Study their chemical properties and reactivity
   Probe the possibility of using them for quantum computing

2) **Computational Catalysis**

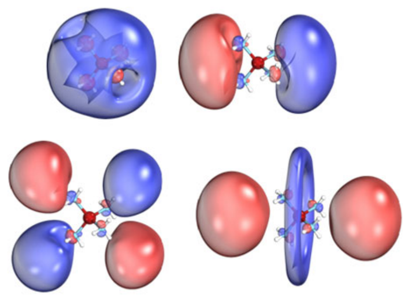
   Catalytic reactions of environmental interest
   - Selective partial oxidation of CH_4 to CH_3OH
   - CO_2 capture and utilization

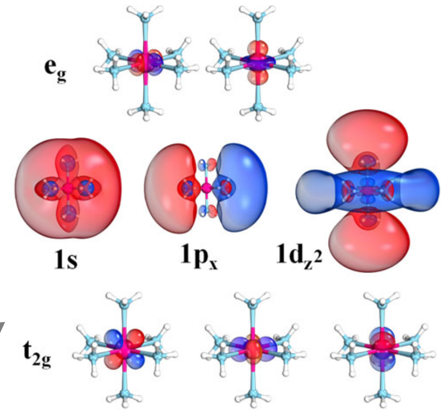
Metal ammonia complexes

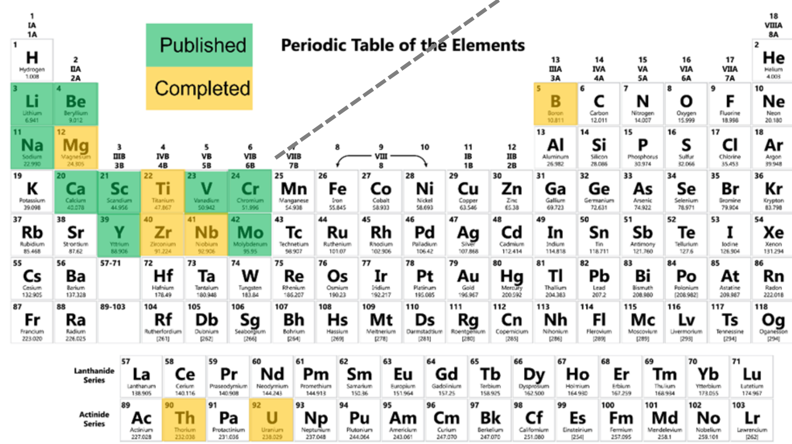
We like unusual systems (SEPs)



$Li^{+}(NH_3)_4$

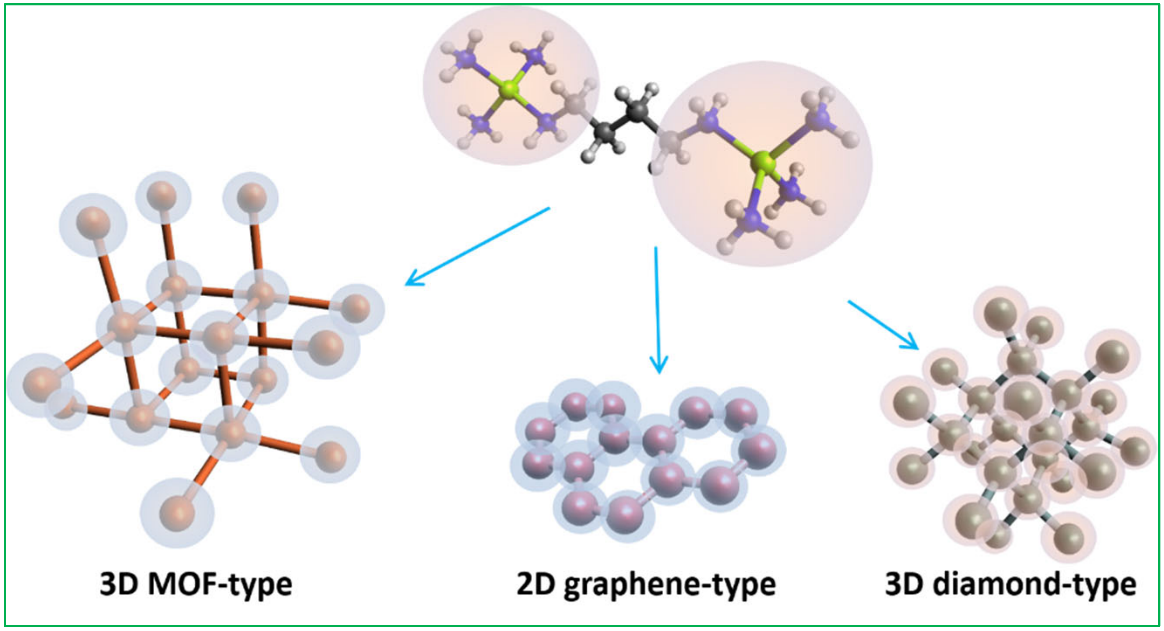






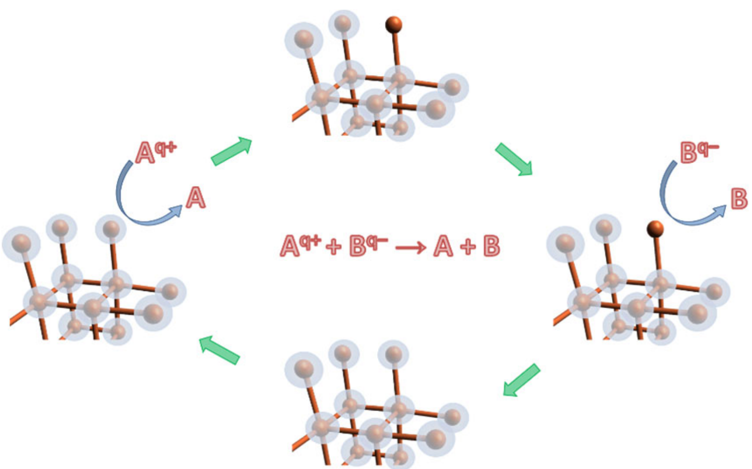
CAREER Award

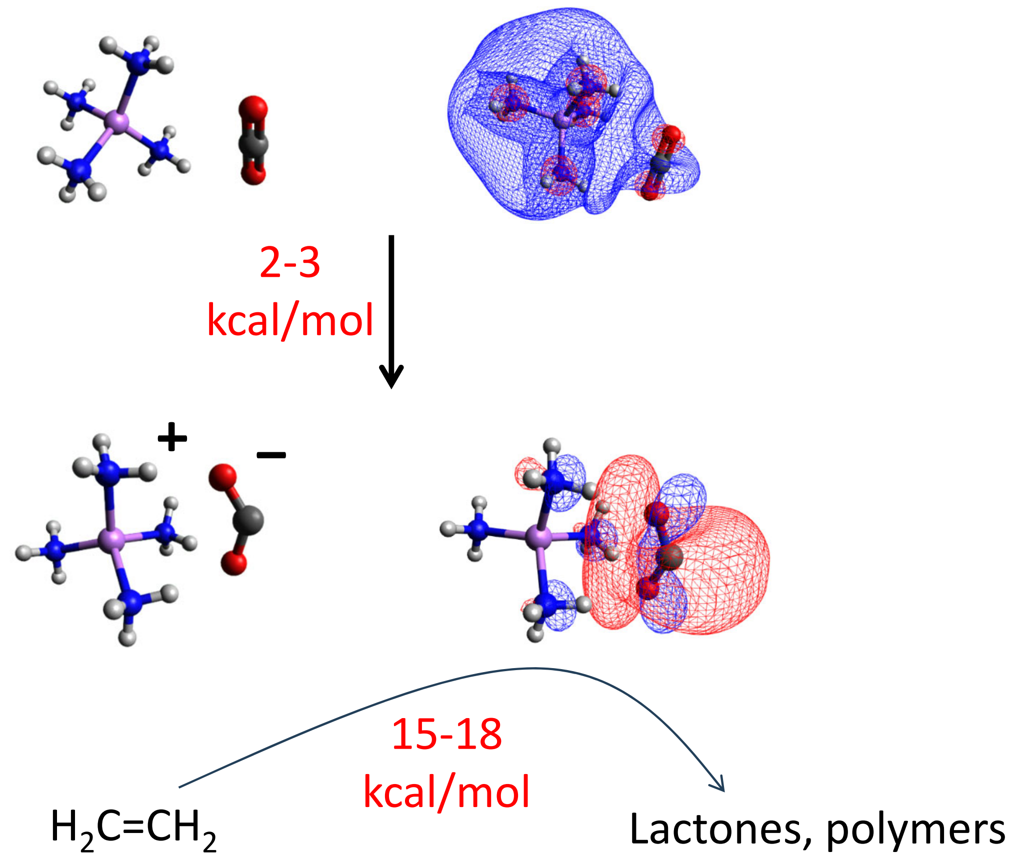
From metal ammonia complexes to novel materials



Application 1: Redox reactions

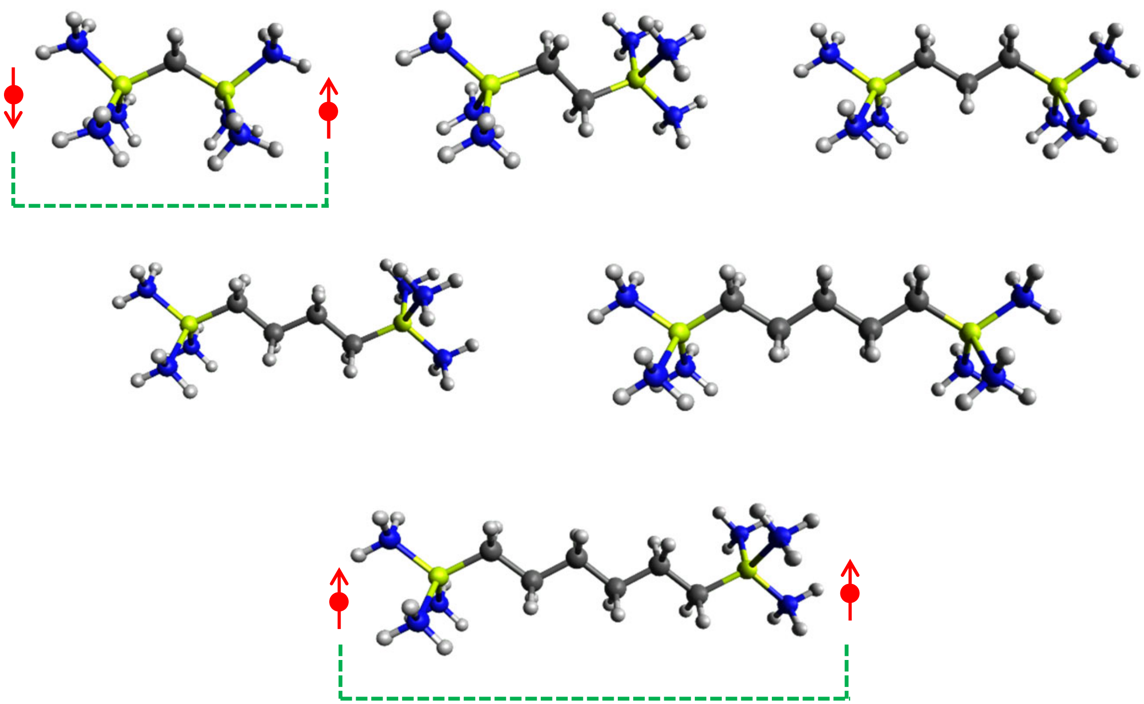
"Birch reduction"





Application 2: Quantum computing

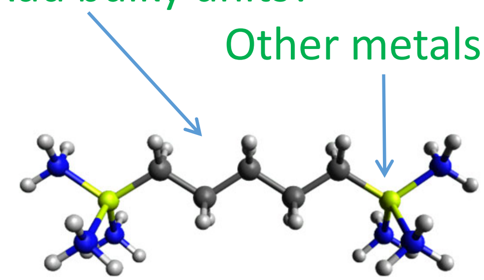
Quantum computing is all about correlation of electrons of neighboring electrons



Add functional groups?

Add bulky units?

Other metals?



Tunable spin coupling and coherence time

Can we tune their properties?

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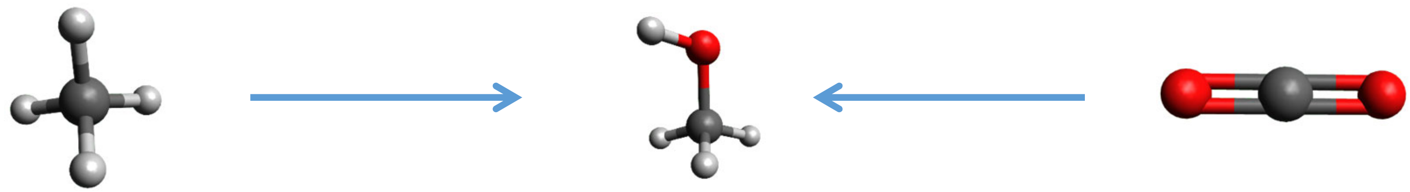
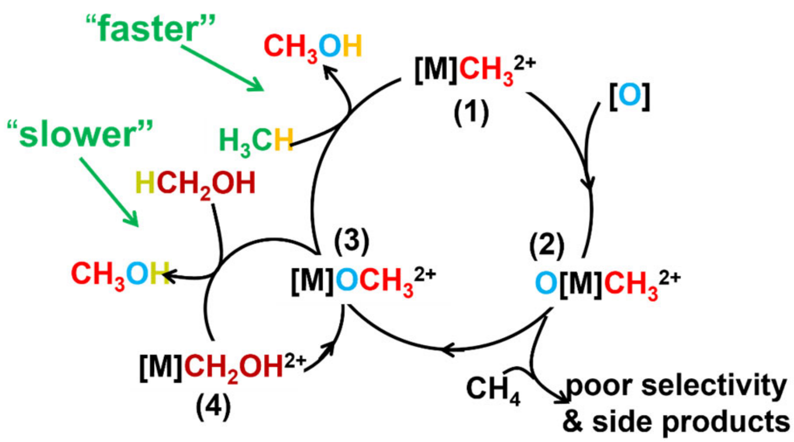
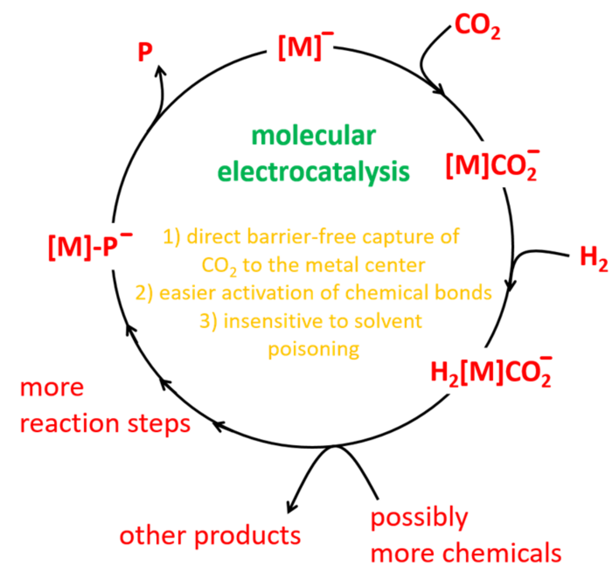
Computational Catalysis





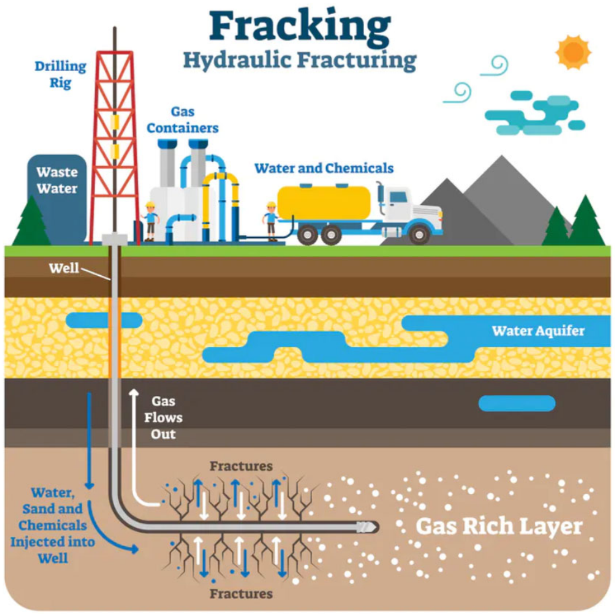


What metal/ligands can do this process better?

<u>Usually two steps</u>

capturing arrangement and catalytic systems

Methane to Methanol transformation. Why this?



CH_4 has become a major hydrocarbon source (natural gas, fracking)
Functionalization is needed for industrial applications (CH_3OH)

Ideally next to the fracking site for cheaper transportation
(CH_4 = gas ; CH_3OH = liquid)

CH_3OH = platform chemical & fuel

EDITOR'S PAGE

The Methanol Economy

This guest editorial is by **George A. Olah,** *director of the Loker Hydrocarbon Research Institute, University of Southern California. A native of Hungary, Olah received the Nobel Prize in Chemistry in 1994 for his pioneering work on carbocation chemistry. He has a long-standing interest in alternative hydrocarbon sources, as well as related energy and environmental issues.*

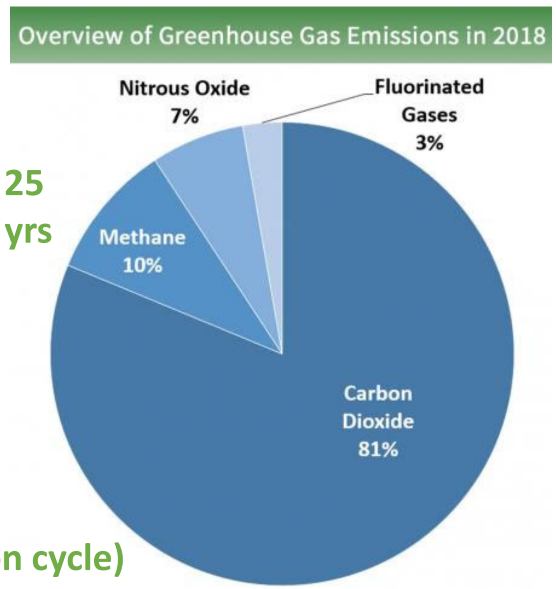
C&EN 81, 38 (2003), DOI: 10.1021/cen-v081n038.p005

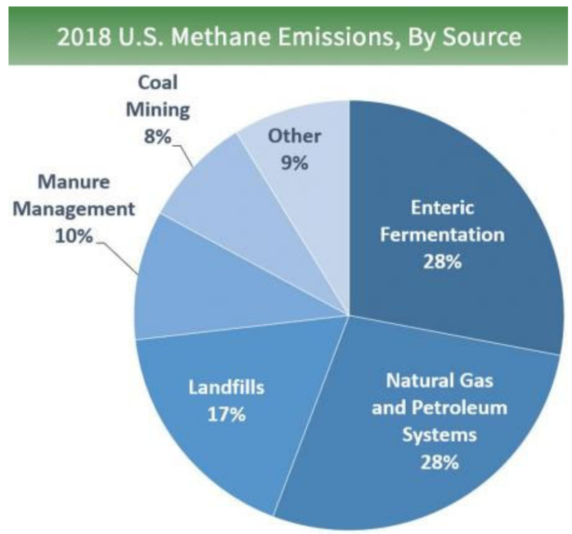
CO_2 and CH_4 = growing atmospheric threats

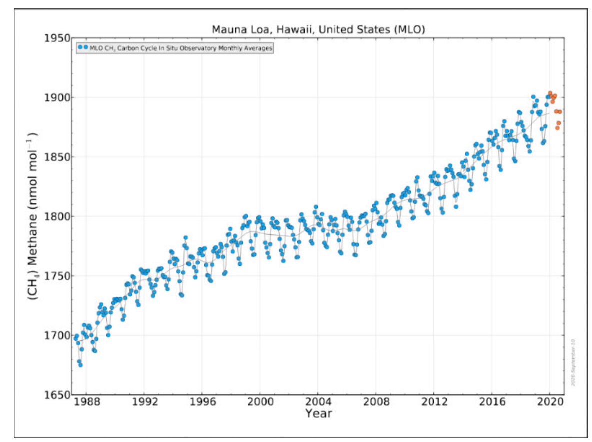
CH_4 and CO_2 have become major atmospheric pollution sources
Capture and utilization will be an ideal solution

GWP = 25
LT = 12 yrs

GWP = 1
LT = 0 – ever
(part of carbon cycle)







*GWP = Global Warming Potential
LT = Life Time

https://www.epa.gov/ghgemissions/overview-greenhouse-gases#methane

Our interests: Check out our review articles

1) **Design of new materials with diffuse electrons**

Study their chemical properties and reactivity
Probe the possibility of using them for quantum computing

https://doi.org/10.1039/D2CP05480A

2) **Computational Catalysis**

Catalytic reactions of environmental interest
Selective partial oxidation of CH_4 to CH_3OH
CO_2 capture and utilization

https://doi.org/10.1039/D3CC02956E

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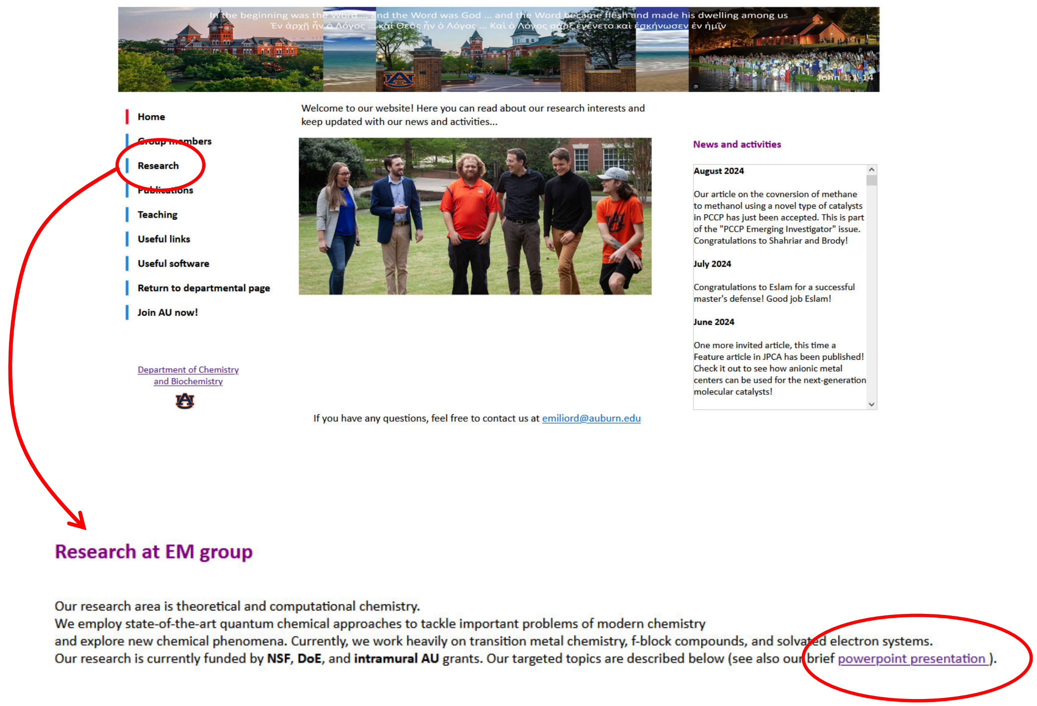

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