

*Miliordos computational chemistry research group*

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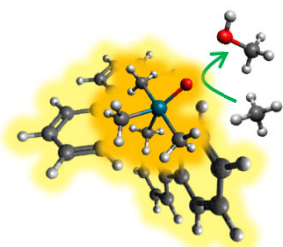
*Auburn, 8/24/2024*

# Miliordos group: Computational Catalysis and Materials with Diffuse Electrons

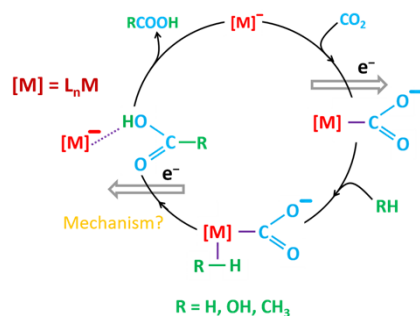
## Computational Catalysis

What is the optimal combination of metal and ligands?

Converting methane to methanol selectively using molecular catalysts

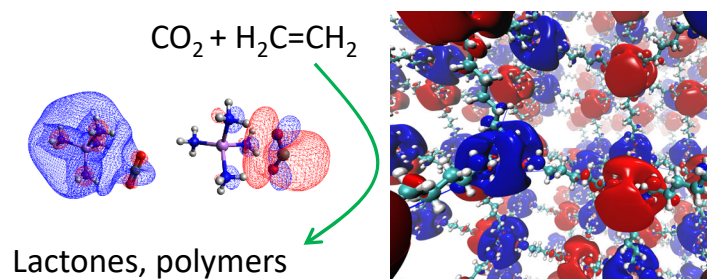


Capture and utilization of CO<sub>2</sub> using transition metal anionic centers

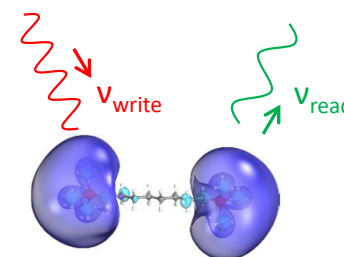


## Chemistry of diffuse electrons

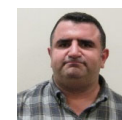
Capturing, reducing and valorizing CO<sub>2</sub>



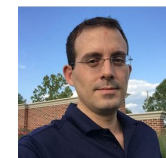
Quantum computing



## Former members



## More info / current members / publications



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# Products and Collaborations

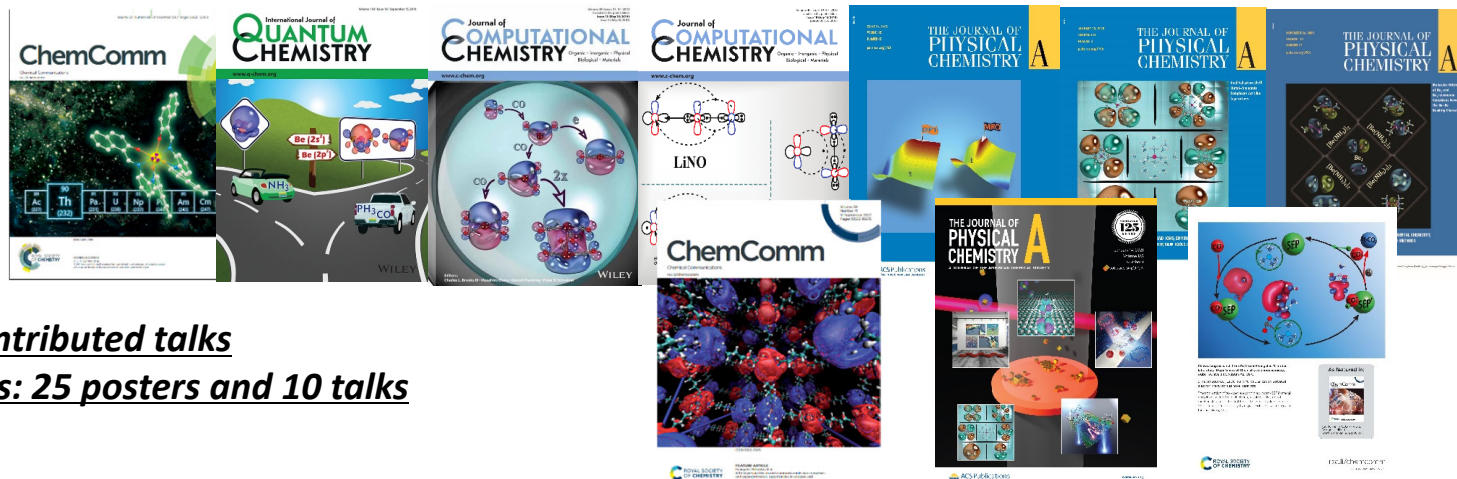
**More than 60 articles over the past seven years (3 highlighted, 10 invited):**

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**

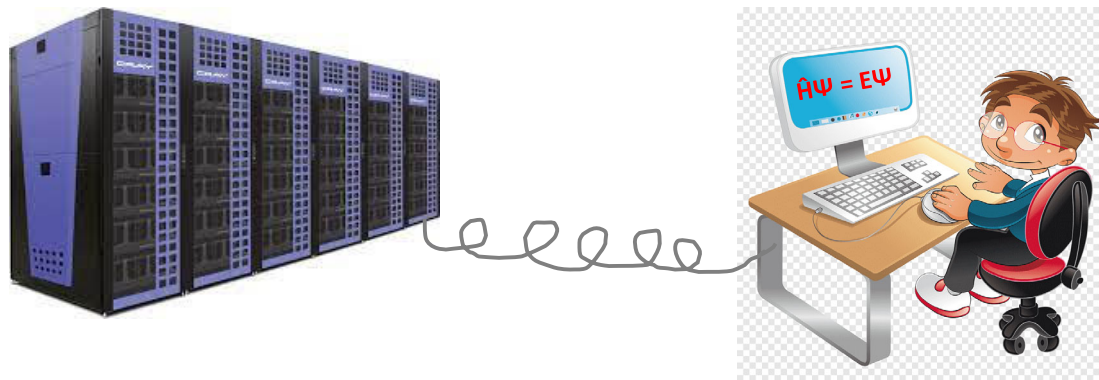
**Students and post-docs: 25 posters and 10 talks**



# We are a computational chemistry group

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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

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## 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

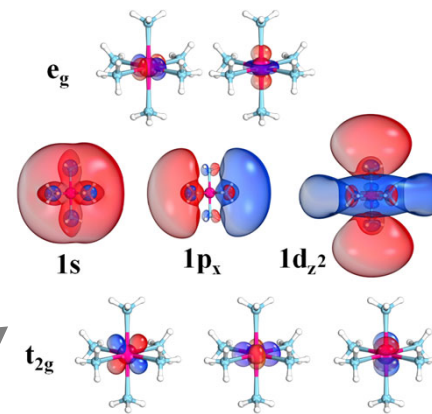
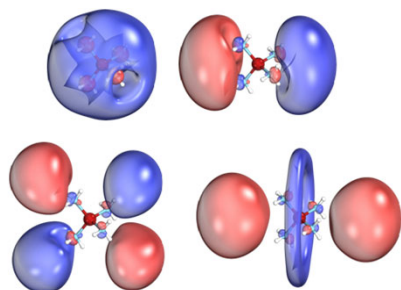
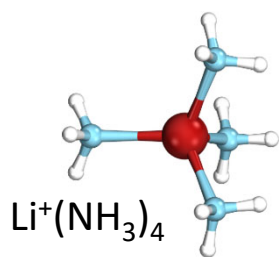
Selective partial oxidation of  $\text{CH}_4$  to  $\text{CH}_3\text{OH}$

$\text{CO}_2$  capture and utilization



# Metal ammonia complexes

We like unusual systems (SEPs)



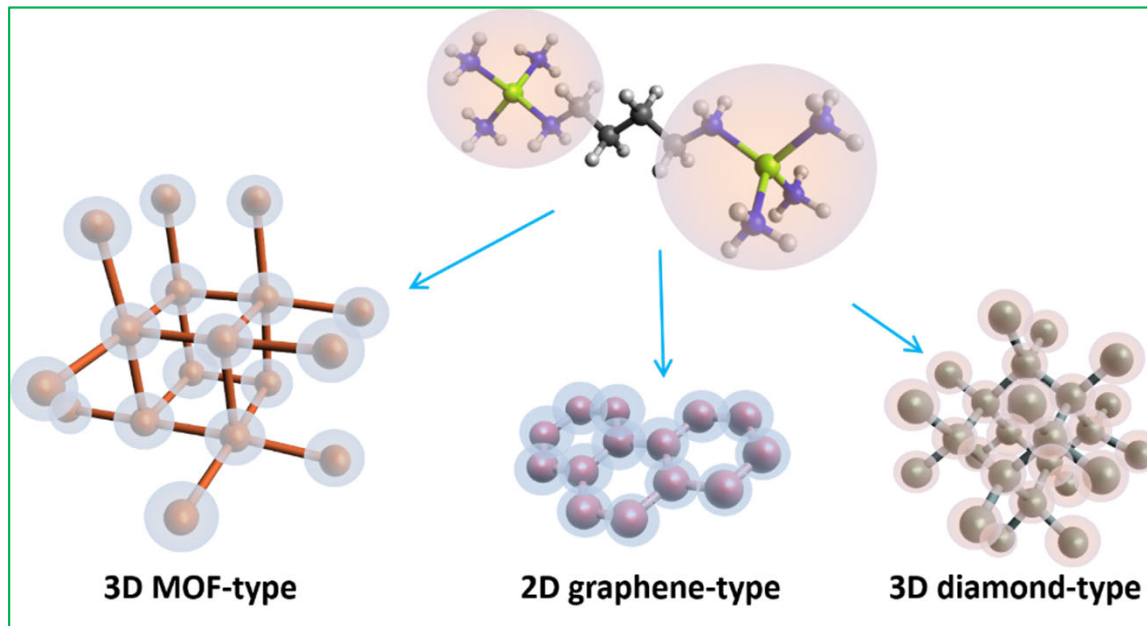
Published  
Completed

Periodic Table of the Elements

1 IA 1A	2 IA 2A											13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A																												
1 H Hydrogen 1.008	2 He Helium 4.003											5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 18.99	10 Ne Neon 20.18																												
3 Li Lithium 6.94	4 Be Beryllium 9.01	3 B Boron 10.81	4 C Carbon 12.01	5 N Nitrogen 14.01	6 O Oxygen 16.00	7 F Fluorine 18.99	8 Ne Neon 20.18											11 Na Sodium 22.99	12 Mg Magnesium 24.31	13 Al Aluminum 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.95																				
19 K Potassium 39.09	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.88	23 V Vanadium 50.94	24 Cr Chromium 51.99	25 Mn Manganese 54.94	26 Fe Iron 55.85	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.38	31 Ga Gallium 69.72	32 Ge Germanium 72.63	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.80											37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium 98.91	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 In Indium 114.82	50 Sn Tin 118.71	51 Sb Antimony 121.76	52 Te Tellurium 127.6	53 I Iodine 126.90	54 Xe Xenon 131.29
55 Cs Cesium 132.91	56 Ba Barium 137.33	57-71 Lanthanide Series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222											87 Fr Francium 223	88 Ra Radium 226	89-103 Actinide Series	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 266	107 Bh Bohrium 264	108 Hs Hassium 277	109 Mt Meitnerium 268	110 Ds Darmstadtium 285	111 Rg Roentgenium 282	112 Cn Copernicium 285	113 Nh Nihonium 284	114 Fl Flerovium 289	115 Mc Moscovium 288	116 Lv Livermorium 293	117 Ts Tennessine 289	118 Og Oganesson 294
Lanthanide Series		57 La Lanthanum 138.91	58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium 144.91	62 Sm Samarium 150.36	63 Eu Europium 151.96	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.05	71 Lu Lutetium 174.97											89 Ac Actinium 227	90 Th Thorium 232	91 Pa Protactinium 231	92 U Uranium 238	93 Np Neptunium 237	94 Pu Plutonium 244	95 Am Americium 243	96 Cm Curium 247	97 Bk Berkelium 247	98 Cf Californium 251	99 Es Einsteinium 252	100 Fm Fermium 257	101 Md Mendelevium 258	102 No Nobelium 259	103 Lr Lawrencium 262				



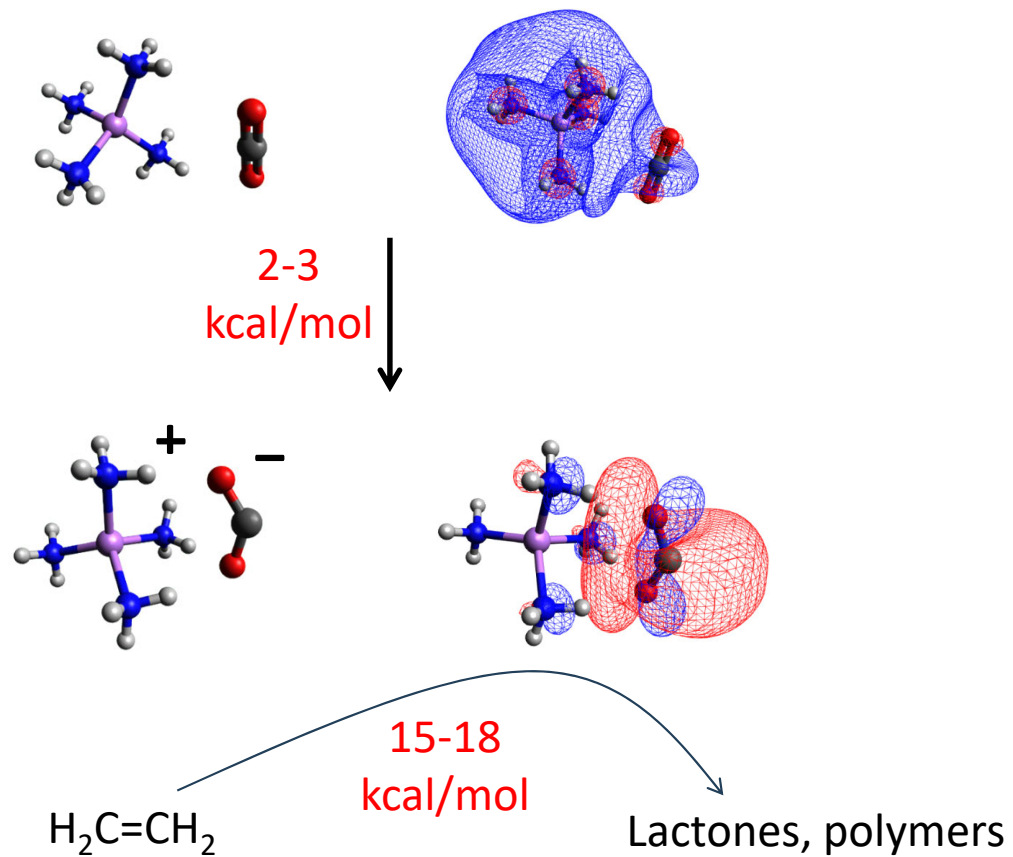
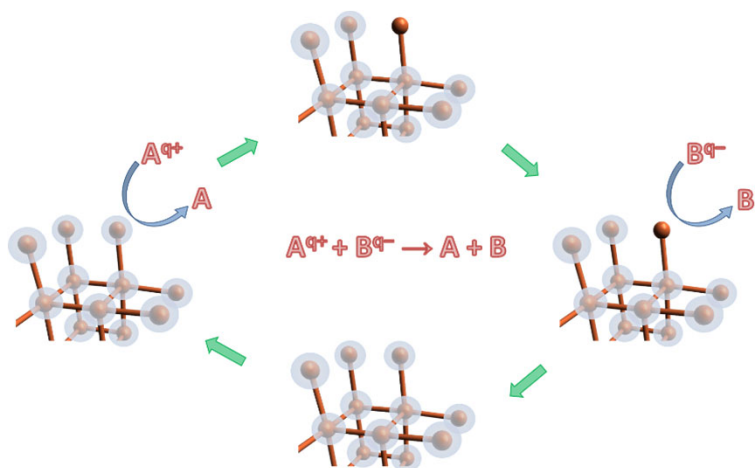
# From metal ammonia complexes to novel materials





# Application 1: Redox reactions

“Birch reduction”

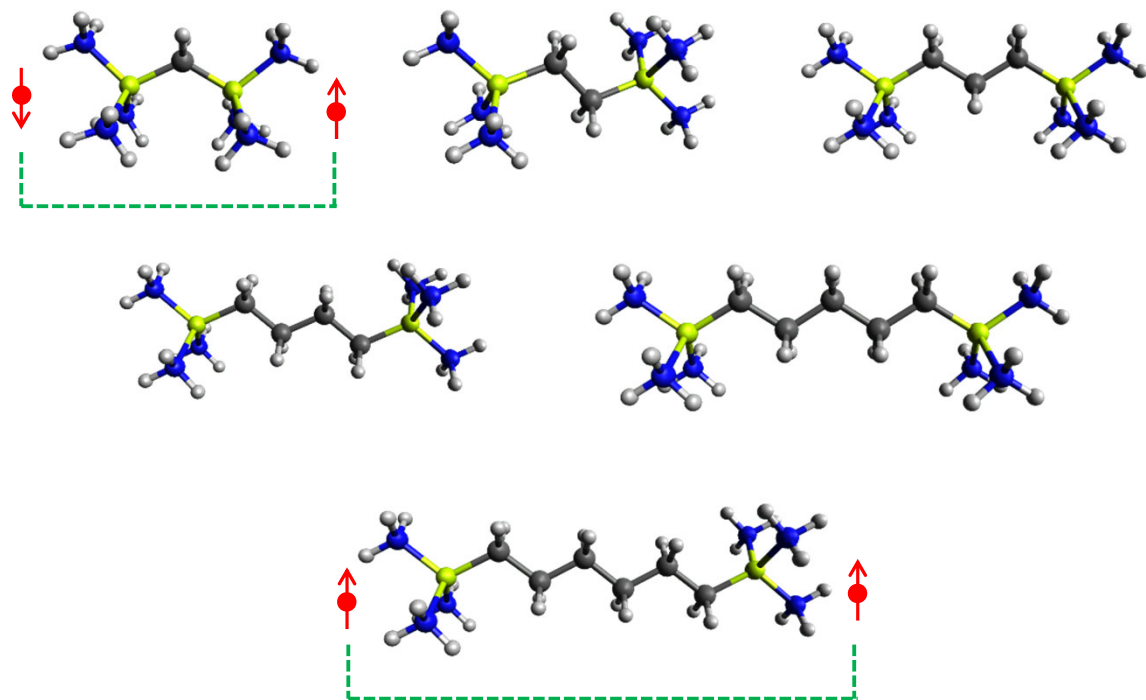






## Application 2: Quantum computing

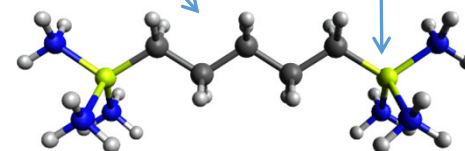
Quantum computing is all about correlation of electrons of neighboring electrons



Add functional groups?

Add bulky units?

Other metals?



Tunable spin coupling  
and coherence time

Can we tune their properties?



# Our interests

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## 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

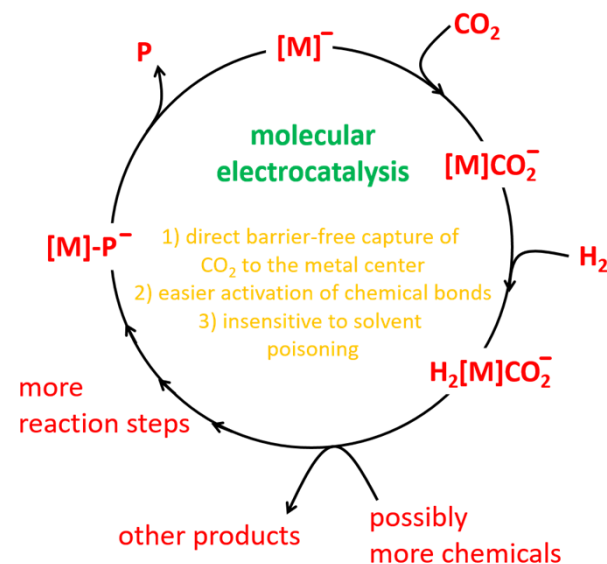
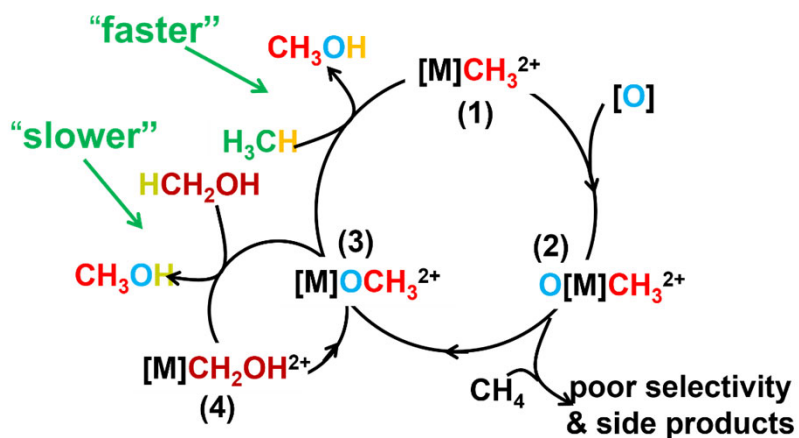
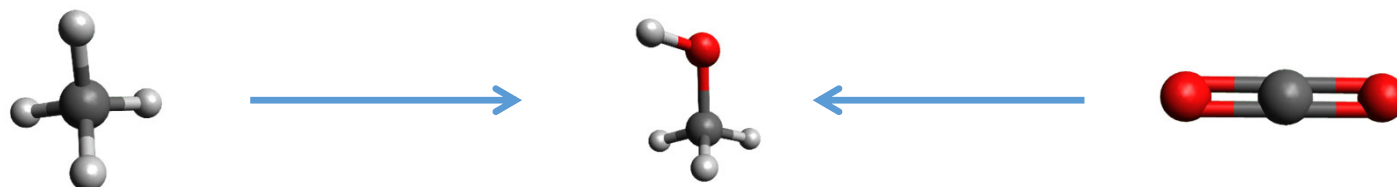
Catalytic reactions of environmental interest

Selective partial oxidation of  $\text{CH}_4$  to  $\text{CH}_3\text{OH}$

$\text{CO}_2$  capture and utilization



# Computational Catalysis



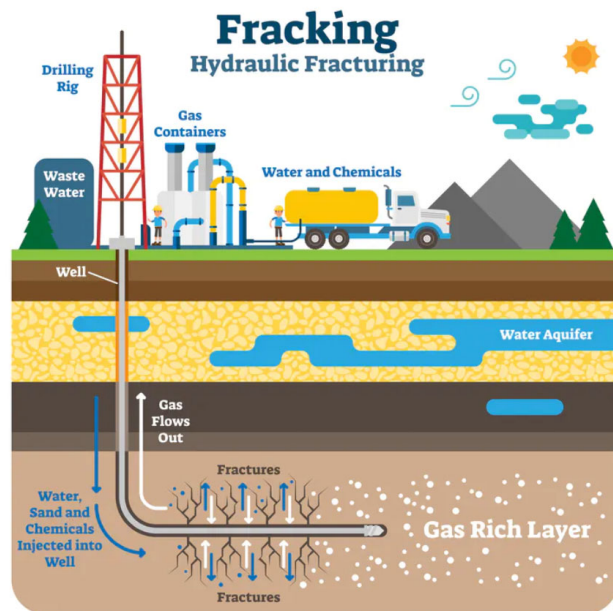
What metal/ligands can do this process better?

Usually two steps

capturing arrangement and catalytic systems



# Methane to Methanol transformation. Why this?



$\text{CH}_4$  has become a major **hydrocarbon** source (natural gas, fracking)  
Functionalization is needed for industrial applications ( $\text{CH}_3\text{OH}$ )

Ideally next to the fracking site for cheaper transportation  
( $\text{CH}_4$  = gas ;  $\text{CH}_3\text{OH}$  = liquid)

**$\text{CH}_3\text{OH}$  = 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.*

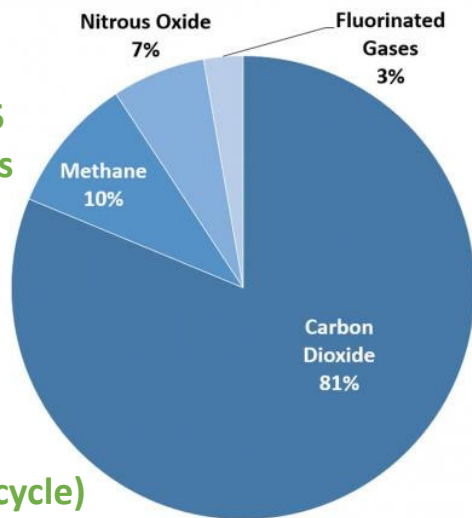
C&EN 81, 38 (2003), DOI: 10.1021/cen-v081n038.p005



# CO<sub>2</sub> and CH<sub>4</sub> = growing atmospheric threats

CH<sub>4</sub> and CO<sub>2</sub> have become major **atmospheric pollution** sources  
Capture and utilization will be an ideal solution

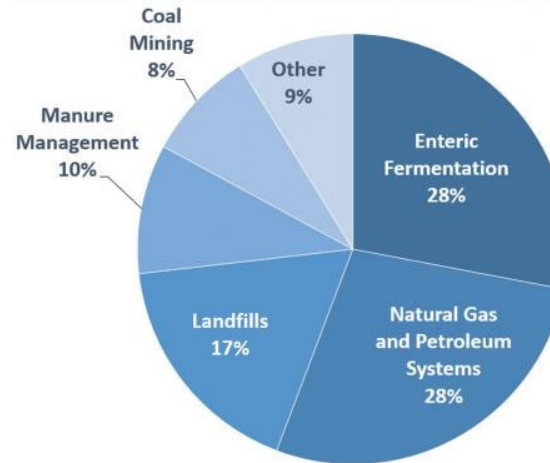
Overview of Greenhouse Gas Emissions in 2018



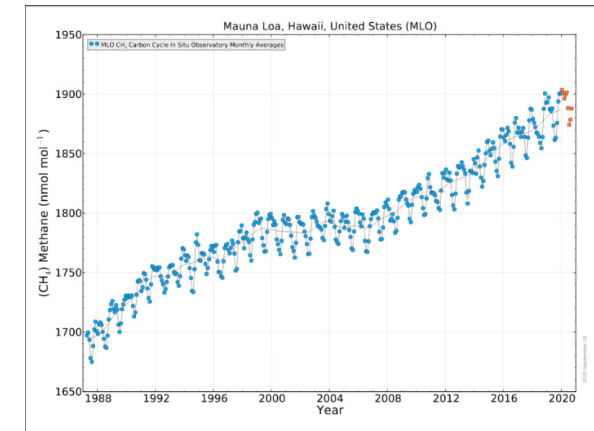
GWP = 25  
LT = 12 yrs

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

2018 U.S. Methane Emissions, By Source



\*GWP = Global Warming Potential  
LT = Life Time



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



## Our interests: Check out our review articles

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### 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  $\text{CH}_4$  to  $\text{CH}_3\text{OH}$   
 $\text{CO}_2$  capture and utilization



<https://doi.org/10.1039/D3CC02956E>

# Miliordos computational chemistry research group

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## Research at EM group

Our research area is theoretical and computational chemistry. We employ state-of-the-art quantum chemical approaches to tackle important problems of modern chemistry and explore new chemical phenomena. Currently, we work heavily on transition metal chemistry, f-block compounds, and solvated electron systems. Our research is currently funded by NSF, DoE, and intramural AU grants. Our targeted topics are described below (see also our [brief powerpoint presentation](#)).

Auburn, 8/24/2024