

COMPUTATIONAL STUDIES IN ASTROCHEMICAL PHYSICS

Summer Research 2020

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<https://blogs.valpo.edu/computational/category/home/>

Summer 2016



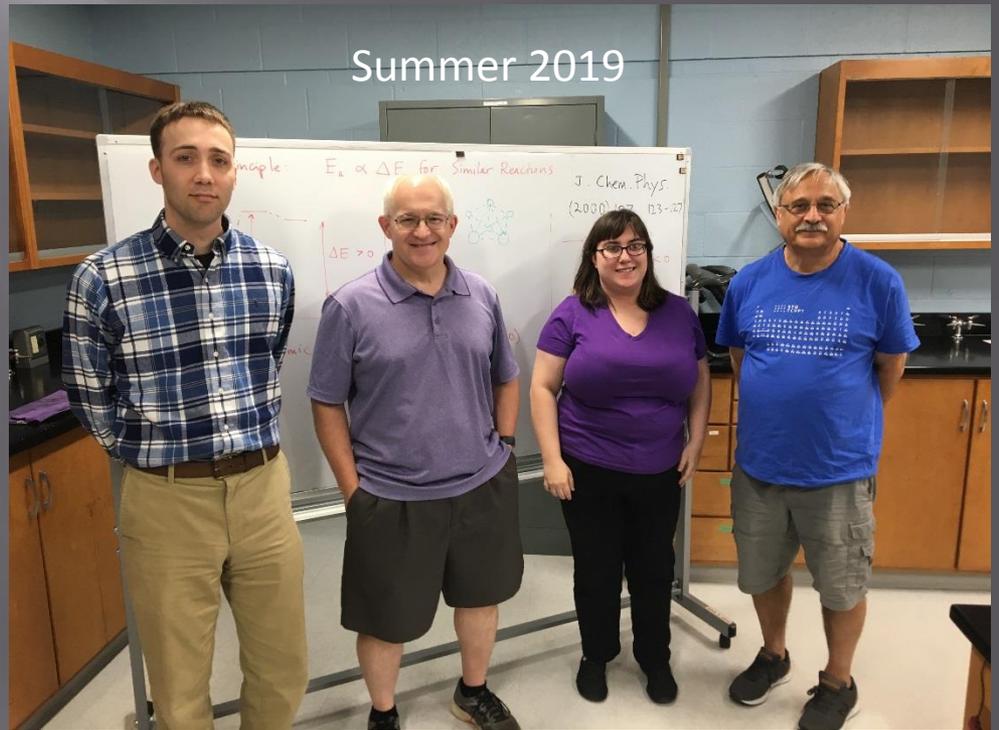
Summer 2017



Summer 2018



Summer 2019



Astronomy + Physics + Chemistry

interstellar medium (ISM)

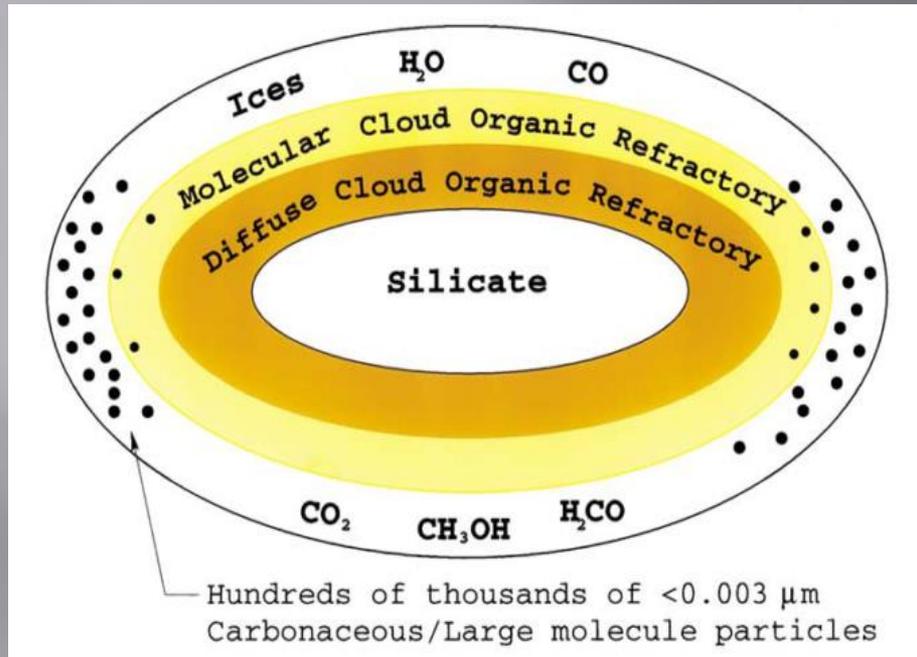


Galaxy M101 as seen in the optical and in the light of atomic hydrogen gas (red)

- ▣ Observation: Many complex organic molecules (COMs) are found in the ISM including polycyclic aromatic hydrocarbons, nucleic acids and amino acids
- ▣ Question: How are these COMs formed?

The goal: better understand star and planet formation and the origins of life

Challenges and Our Approach



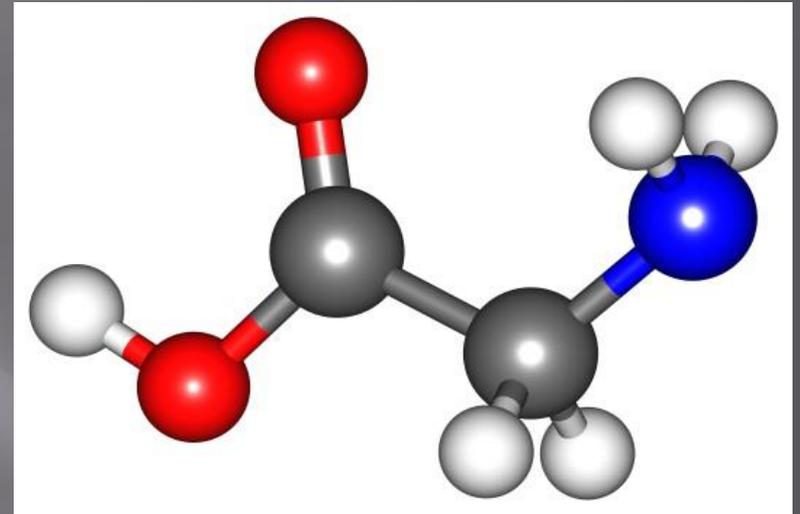
A typical dust grain

- ▣ ISM contains mix of matter and radiation (EM, cosmic rays)
- ▣ The dust (1% of ISM) contains the largest and most complex organic molecules
- ▣ $T \sim 5-10 \text{ K}$

The method: use computational quantum mechanics to study photochemical radical reactions

Project I: Formation of Glycine in Interstellar Space (Prof. He)

- ▣ Radical production and combination
- ▣ Different environments: the gas phase, the modelled ice, and a graphene surface
- ▣ Primary Steps



Structure of glycine (one type of amino acid)

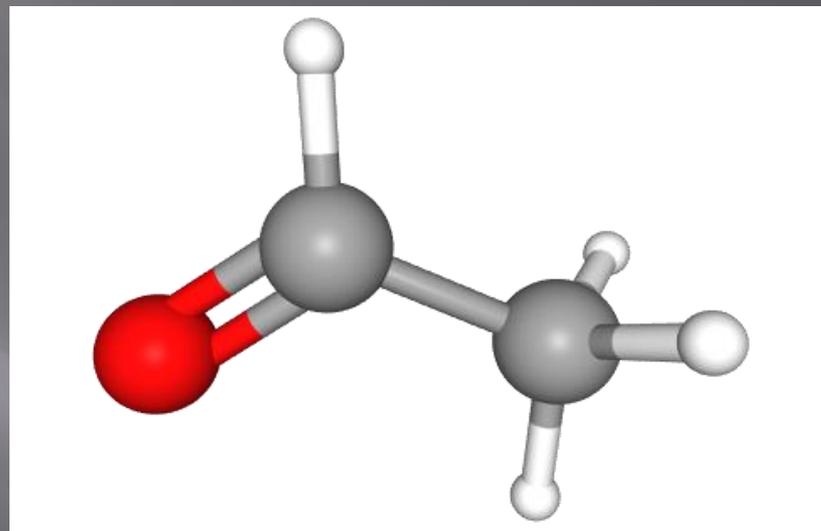


Project II: Formation of Acetaldehyde in Interstellar Space (Prof. Zygmunt)

- ▣ Radical production and combination to form C-C bond
- ▣ Different environments: the gas phase, the modelled ice, and a graphene surface
- ▣ Proposed Reaction



At low T, does this happen in gas phase or on a dust grain surface?



Structure of acetaldehyde (test case for more complex COMs)

Summer Research Internships

- ▣ 2 students will be hired subject to availability of funding
- ▣ 8-10 weeks in summer, 30-40 hours per week
- ▣ The students will learn to use electronic structure codes to run calculations, analyze data and report results in both oral and written formats. The student will be required to create a poster presentation and submit a report at the conclusion of the summer
- ▣ All UG students are eligible to apply