# Honors Thesis

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# Abstract

The general idea of this iterative process is to train ZeoGAN to produce crys- talline porous structures with low energies from the energy values obtained from HydraGNN. The input configuration for HydraGNN is in Cartesian coordinates format, while the output of ZeoGAN is the crystal lattice infor- mation of a materials' grid, specially the probabilities an atom exists at every coordinate in the unit cell. Thus, in order to integrate the HydraGNN as a function within ZeoGAN and form this iterative process, the output of ZeoGAN must be converted into this Cartesian format. My primary assign- ment was to develop an algorithm which can be implemented in ZeoGAN to accurately do this conversion and will be used to train HydraGNN. I am also working on creating visualizations of the 3D molecular structures to confirm and assess the accuracy of the material grids of the structures generated from ZeoGAN, which is difficult to do with only the given data.

Expanding and combining the efforts of two recently developed algorithms

# 1 Introduction

The most pressing issue facing the global community is climate change and global warming, which has instigated the re-examination and discussion of concerns regarding current energy and fuel resources. Cutting-edge technology and machine learning have enabled new discoveries and improvements on existing solutions to this imminent crisis, such as new and innovative methods of capturing greenhouse cases.

Recent research points to prioritizing the capture, storage, and use of methane emissions as a potential solution to the fuel crisis. The removal of methane can lead to significant improvements in overall air quality and decreases in global warming since it is the second most abundant greenhouse gas and extremely potent in trapping heat (Jordan, 2021). The combined risk factor associated with methane's high flammability and lack of existing research on methane capture and energy efficient conversions to fuel makes it challenging to safely work with. However, it offers promising potential to be a source of energy that surpasses other fossil fuels as a solution to the fuel crisis. Furthermore, significant removal of methane can lead to drastic decreases in overall global temperatures and the issue of global warming since methane is the direct contributor to an increase in the tropospheric ozone layer (Jordan, 2021).

Zeolites, a class of crystalline, microporous inorganic solid consisting of silicon and oxygen atoms, offer a safe and reliable solution to storing and transporting methane and other volatile gases, such as carbon dioxide, without further emitting pollutants. This research focuses on combining and improving existing algorithms for inorganic solids design of 3D atomic-scale periodic structures of zeolites. The merge of the generative adversarial network, ZeoGAN, and a multi-tasking graph convolutional neural network model, HydraGNN.

ZeoGAN, or zeolite GAN, is an existing basic GAN model with the goal of generating crystalline porous nanomaterials and energy shapes using artificial neural networks, while HydraGNN predicts global and atomic physical properties given atomic structures. Using a high-performance organization procedure, The integration of HydraGNN as a function within the ZeoGAN algorithm allows for the generation of new atomic structures with low energies or any optimization of user-desired properties.

This research is conducted in conjointment with the AI Initiative in the Department of Computational Chemistry and Nanomaterials Sciences at Oak Ridge National Laboratory. (ask Dr. Irle what credits need to be added?)

# 2 Literature Review

Global warming and climate change have become immediate concerns that have led to many insolvable problems that we seek to solve through other alternatives as well as new age technology. It is not only important to discover better methods of capturing greenhouse gases, but also critical to uncover and develop new technologies to create better alternatives for the fuel economy.

## 2.1 Methane

Methane is one of the most prioritized greenhouse gases. It is the second most abundant greenhouse gas after carbon dioxide. Concentrations of methane emissions have grown more than twice as fast as carbon dioxide due to human-related activities since the Industrial Revolution and is 81 times more potent at trapping heat in its first 20 years of release (Jordan, 2021). Primary causes are from agriculture, waste disposal, and fossil fuel extraction. However, there are also natural sources of methane that account for 40% of global methane emissions. Focusing efforts on significant reducing methane emissions would absolutely be influential on global warming and its potential to be exacerbated. Removal of methane will be beneficial to improvements in air quality as well since the oxidation of methane is the primary contributor to the formation of the ozone layer in the troposphere (Jordan, 2021).

Methane also has the highest potential to solve our current fuel crisis. In comparison to other hydrocarbons, it is more environmentally beneficial because it produces more heat and light energy by mass, while emitting significantly lower than carbon dioxide.

The recent discovery of methane clathrates, or more colloquially known as “fire ice”, are sources of high energy-intensive fuel found as an ice crystal (Yoon, 2017). Methane clathrates are formed through a combination of low temperatures and high pressure and contain locked reserves of natural methane gas. One cubic meter of the compound releases about 160 cubic meters of gas (S.-Y. Lee & Holder, 2001). These enormous deposits of methane can be found distributed throughout permafrost regions and soil microbes in wetlands with more energy stored in methane hydrates compared to the world’s oil, coal, and gas combined (Yoon, 2017). Recent efforts to convert this methane gas to energy has proven to be fruitful. Thus, despite environmental and global warming concerns, plans have been made to make methane a leading source of alternative energy in the future to other fossil fuel sources (Yoon, 2017).

[another potential way it is a fuel solution (?) – conversion to syngas]

There has also been a lack of development of technology for methane removal due to challenges related to its concentration and dilution is extremely low (Lackner, 2020). A known way to use methane is to convert it to methanol, a liquid form of fuel that burns more cleanly with fewer emissions. However, this conversion process requirees significant heat and pressure, which generates a significant amount of carbon dioxide emissions. In addition, storage, transportation, and utilization of methane presents its own set of problems. Methane is highly flammable and has a high risk of combustion - making it a difficult greenhouse gas to safely manipulate (Yoon, 2017). Improper handling of methane poses danger of exacerbating current global warming issues. The current trajectory of global warming is melting permafrost regions with methane hydrates, which could result in the release of trillions of cubic meters of methane into the atmosphere (Yoon, 2017). This risk and the current lack of existing research and resources to capture methane in a reliable and energy efficient manner makes it difficult and dangerous to handle.

New technology and research has discovered a class of crystalline, porous material capable of safely and stably soaking up, captuing, and storing methane gas called zeolites (Jordan, 2021). Zeolites hold the promise of a solution to many of the environmental issues facing our world, including but not limited to methane and carbon dioxide capture and storage.

## 2.2 Zeolite

## 2.3 ZeoGAN

## 2.4 HydraGNN

# 3 Methods

- flood fill algorithm

# 4 Results

results....

# References


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