

LEAP24 AI Oasis Hackathon



# **Virtual lab** for Advanced Material development

# You know what, We will present our idea with a small story 😊

In 2020, as a new virus spread globally, **X-Company**, a leading pharmaceutical firm, sprang into action. Despite pouring resources into research and experimentation, time-consuming, progress remained sluggish, costs soared, and rapid experiment failures led to waste and unnecessary expenses 🙄.

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Meanwhile, their rival, **Company-Y** 😎, was so lucky by employing **EMXOR**, a virtual lab platform. Leveraging AI and conducting virtual experiments, design and more in the cloud, Company-Y dramatically reduced development timelines and costs. In record time and with minimal resources, they discovered the most effective drug to combat the virus 🎉🎊🎊.

This victory highlighted the transformative power of integrating advanced technologies. By leveraging **EMXOR**, Company-Y sidestepped common pitfalls in material development, ensuring swift progress and cost efficiency in their quest for solutions.

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# The Problem

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- Creating or developing advanced materials involves high R&D costs. The global annual spending on materials science R&D *surpasses \$100 billion*.
- Lengthy Development Timelines: It takes *an average of 10 to 20 years* to bring a new material from initial discovery to commercialization.
- Technical issues often lead to about *80% of advanced materials projects failing* to achieve their goals.

# The Solution

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**Meet our Platform:** *Your cloud-based **virtual lab and research center** where you can do Experiments, prediction generating & optimizing molecules to enhance the development of advanced matter...*

**Using cutting edge** We leverage **AI** and integrate existing CLM, LLM and cloud computing technologies to predict the product of a reaction, plan synthesis and more. Converting molecule structure into SMILES strings and input them into *CLM model* to do desired task...

# Business Value

Our platform provides a cloud-based virtual lab for companies like Pfizer and Nvidia, *speeding, reducing time/cost and enhancing better R&D* by predicting and optimizing molecules. This reduces costs and shortens the typical **10-20 year** development cycle, leading to more **successful projects and faster innovation.**



# Market Opportunity

**\$513B**

2023 ~ Global Advanced  
Materials Market Size

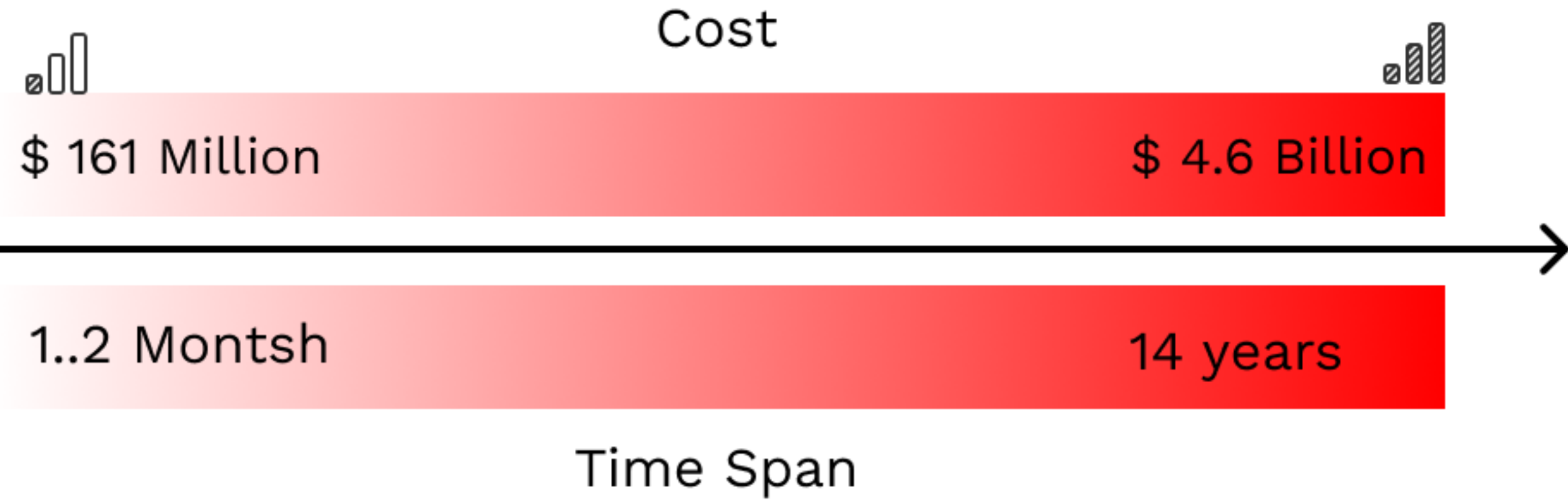


**\$695B**

USD 695.5 Billion by 2028, at  
a CAGR of 6.2% from 2023 to  
2028



# Without EMXOR Traditional Development and R&D of Material e.g. Drug



reduce  
by 70%

# With **EMXOR** Reduce By 70%



## Client Input

Text  
SMILES  
Graph ~ Draw

Encoder/Decoder  
+ Backend  
(microserver)

Help with  
Model  
Inputting and  
converting

Assigns Task and  
CLM Module's

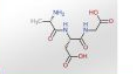
Molecule Optimization  
Tet conditional de novo generation  
Retrosynthesis  
Chemical reactions  
Product prediction  
Molecule Optimization

event driven architecture

CLM Output



Optional Graph



OpenAI  
GPT-4  
LLM Description

# Architecture



Serving AI driven models to help with the development of material

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AI-ML



Converting Molcluel graph into SMILES to do chemecil computation on it like (predction, retrosynthetic analysis)

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CLM



GPT - 4

Large language model

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LLM GPT-4



Google Cloud

Google cloud to empore our platform

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CLOUD GCP

# Tools and Technology



Currunlty we integrate intelgent CLM models to help us constructing the lab

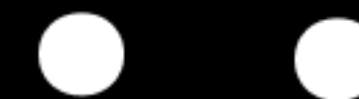
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Integrating Intelligence Model

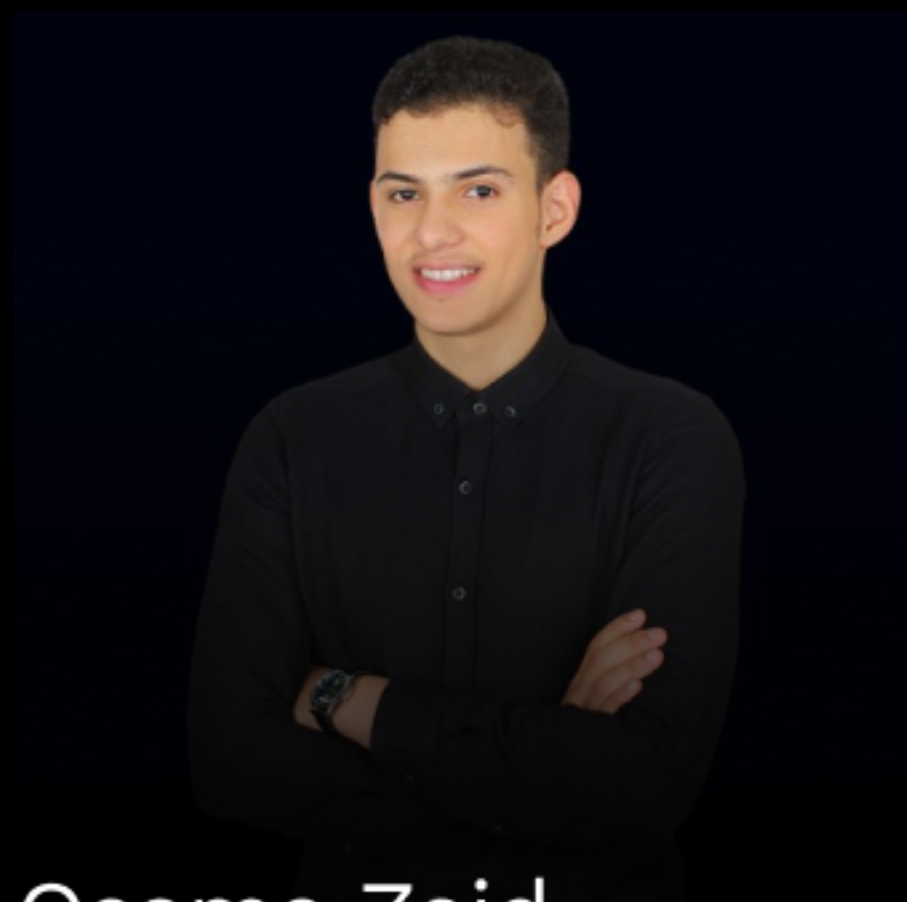
ChemDoodle 2D contains thousands of chemistry features, helping you produce the highest quality graphics and saving you hours of work.

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ChemDoodle Framework



# Team



Osama Zaid

Software-ML Engineering

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Eslam Zaid

Software engineering

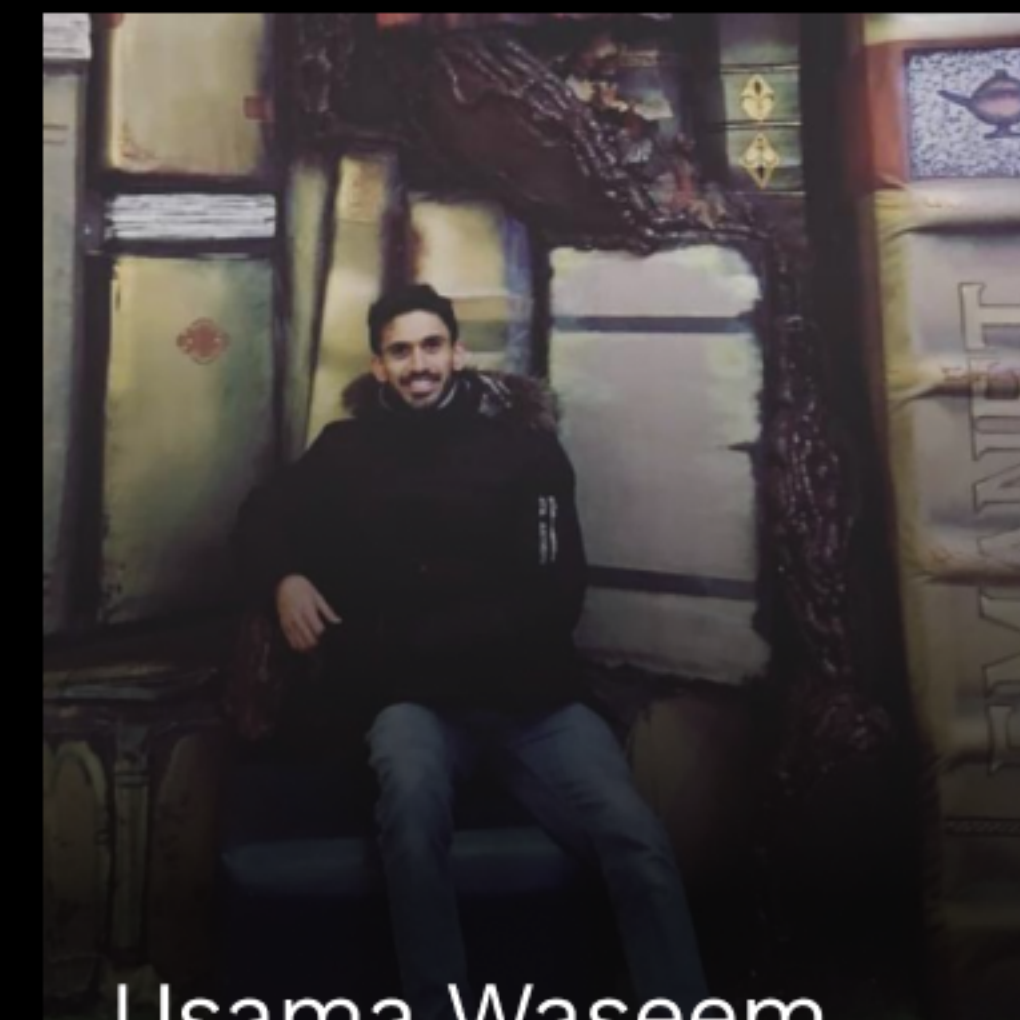
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Ahmed Alzahrani

ML Engineer

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Usama Waseem

Artificial Intelligence

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**THANK YOU**

