QCROP

قيو كروب

12 RESPONSIBLE CONSUMPTION AND PRODUCTION

13 CLIMATE ACTION

PROBLEM

The Haber-Bosch Process is **unsustainable.**

1.5% of global CO_2 emissions.

1% of global energy consumption.

12 RESPONSIBLE CONSUMPTION AND PRODUCTION

13 CLIMATE ACTION

PROBLEM

The Haber-Bosch Process is **unsustainable.**

260 million car emissions.

15x energy consumption of UAE.

SO... JUST ABANDON IT?

Well - we can't.

50%

of world's food production
is dependent on fertilizers

9 INDUSTRY, INNOVATION AND INFRASTRUCTURE

SOLUTION

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Improve the efficiency of fertilizer production by optimizing the process using quantum molecular simulation.

VALUE ADDED

To the public

- Reduced environmental harm
- Sustainable future
- Open Source Project

To the customer

- Efficient & sustainable fertilizer production
- Valuable insights into catalytic reactions
- Optimized reactions for improved yields and reduced waste

APPROACH

- VQE
- Error Mitigation
  - Zero Noise Extrapolation
  - Measurement Error Mitigation

PLATFORMS

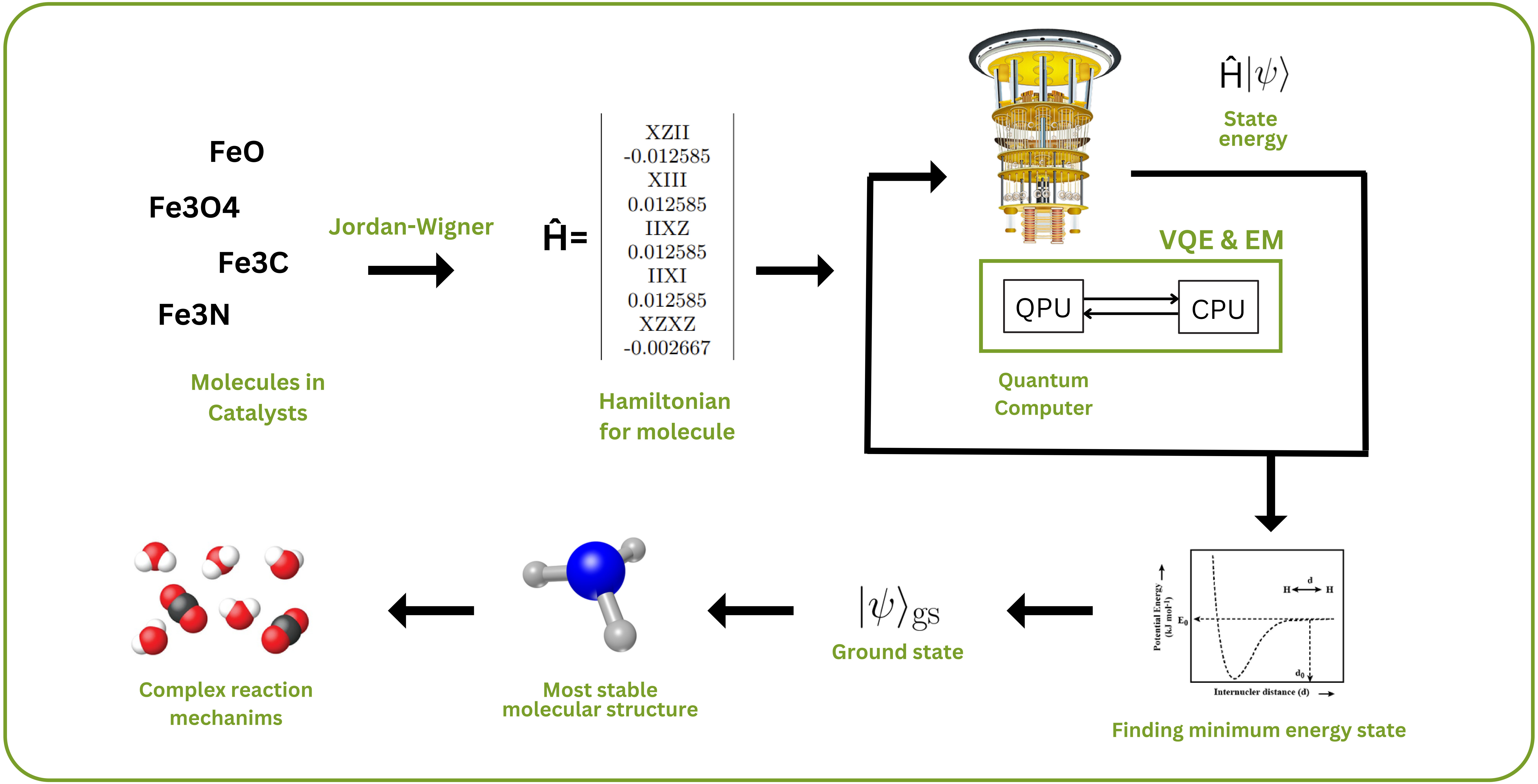
React

qBraid

IBM

Qiskit

SYSTEM ARCHITECTURE



PRODUCT

```
!pip install qcrop
```

```
import qcrop
```

Python Package

Web App

https://github.com/ro1406/QCrop

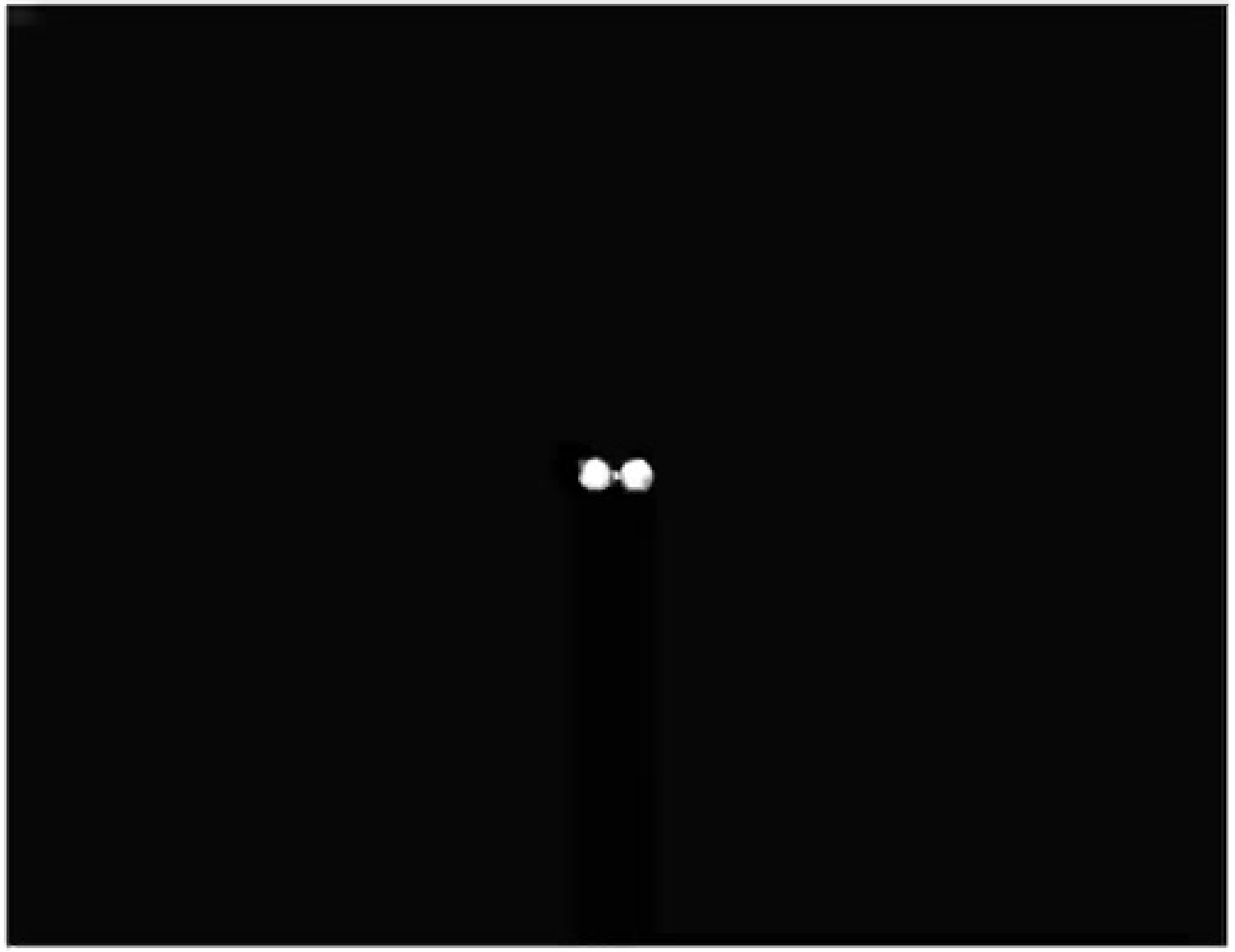
WEB APP

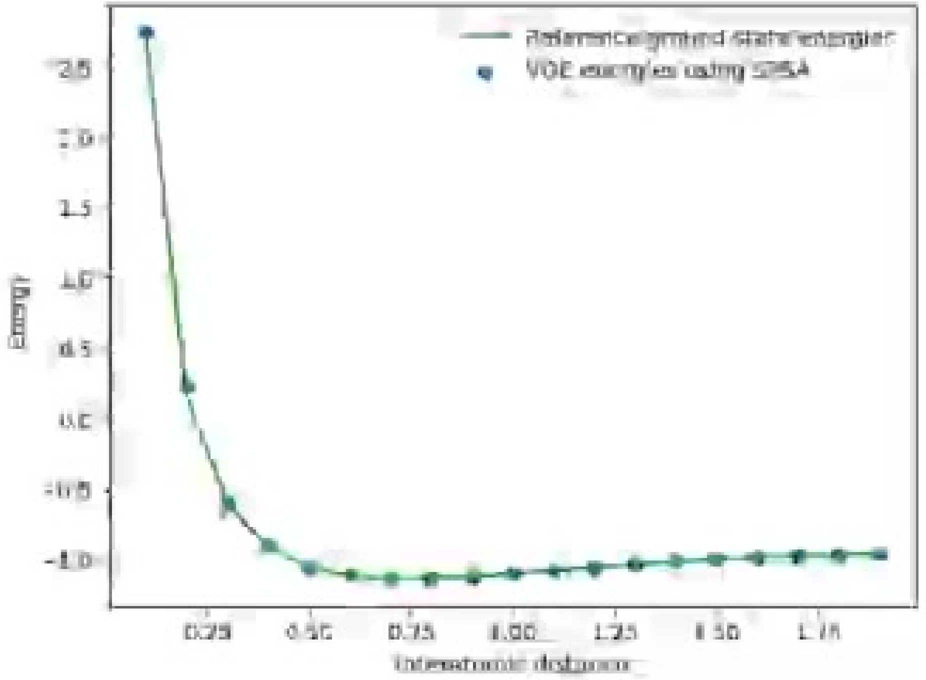
DEMO

Home About

H2 BeH2 LiH

Analysis Result of Hydrogen (H2)





Select Interatomic Distance VQE Result: Exact Energy:

CUSTOMER SEGMENT

Fertilizer Manufacturers

Crop Research Facilities

Early Adopters

We discussed our product idea with

OCP

MARKET SIZE - CATALYSTS

USD 39.45 Billion
2022

USD 61.82 Billion
2030

CAGR
5.77%

Fragmented Market

Source: Precedence Research

BUSINESS MODEL

Pay-for-performance

We get paid for each percentage point improvement

WHY QUANTUM?

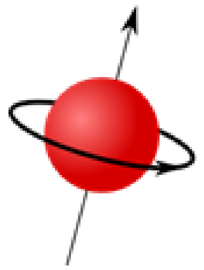
“Nature isn't classical... and if you want to make a simulation of nature, you'd better make it quantum mechanical... and by golly it's a wonderful problem, because it doesn't look so easy.”

Richard Feynman

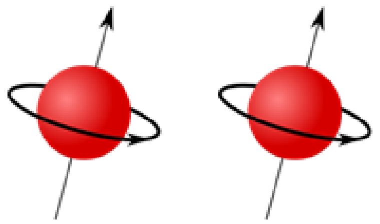
WHY QUANTUM?

Resource requirement grows exponentially on classical computers.

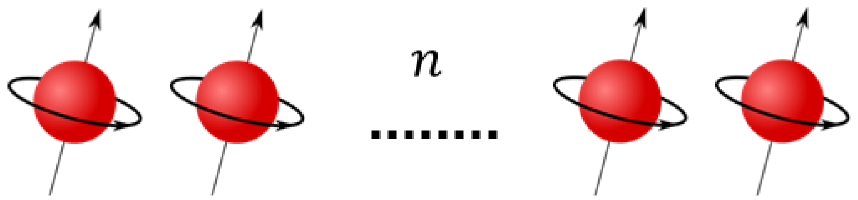
$$O(2^n)$$



$$|\psi\rangle = c_1|\uparrow\rangle + c_2|\downarrow\rangle$$



$$|\psi\rangle = c_1|\uparrow\uparrow\rangle + c_2|\uparrow\downarrow\rangle + c_3|\downarrow\uparrow\rangle + c_4|\downarrow\downarrow\rangle$$



2^n superposition states!

CONCLUSIONS

Successfully harnessed the power of Quantum Computing to...

Cater to growing demand of sustainable production

Gain deeper insights to catalyst reactions

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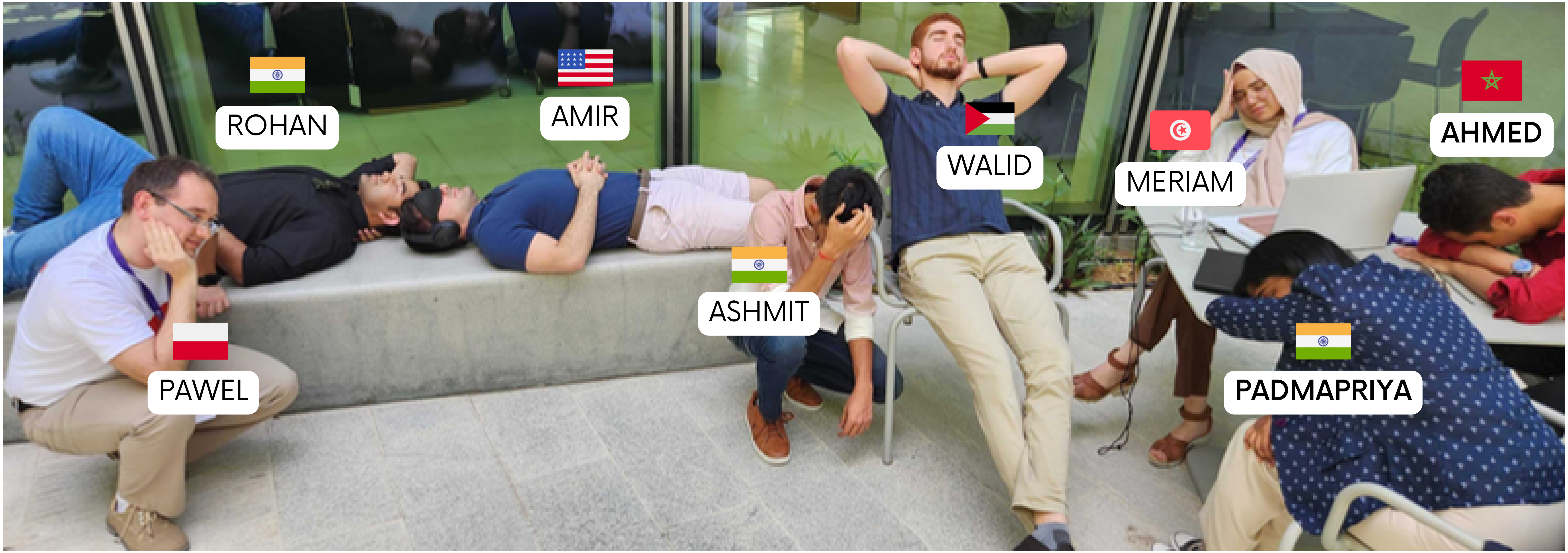
Optimize reactions for sustainable fertilizer productions

Harbor a sustainable future

THANK YOU

We've reached our ground state too.



Appendix

References

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Kandala, A., Mezzacapo, A., Temme, K. et al. Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. Nature 549, 242–246 (2017). https://doi.org/10.1038/nature23879

Baiardi, A, Christandl, M., Reiher M., Quantum Computing for Molecular Biology. https://doi.org/10.48550/arXiv.2212.12220

https://mitiq.readthedocs.io/en/stable/apidoc.html
https://qiskit.org/documentation/

Closest competitors

(they do general molecule simulations but don't focus on fertilizers)

- **EUMEN**
- **Molecular Quantum Solutions**
- **HQS**

Why is ground state important?

- **Determines the most stable electronic and geometric structure of the molecule, which in turn affects the reactivity and selectivity of the catalyst.**

- **In a chemical reaction, the reactants must overcome an energy barrier (activation energy) before they can form products. The ground state of a molecule is the state of minimum energy, which means that the molecule is in its most stable configuration. If the reactants can reach this stable configuration, they are more likely to form product.**

- **Electronic structure of the molecule in its ground state can affect the binding strength between the reactants and the catalyst. The strength of the interaction between the reactants and the catalyst can affect the rate of the reaction and the selectivity of the products.**

Insights obtained from ground state

- Relative energies of stable configurations
- Prediction of complex reaction mechanisms