Chemical fertilizers

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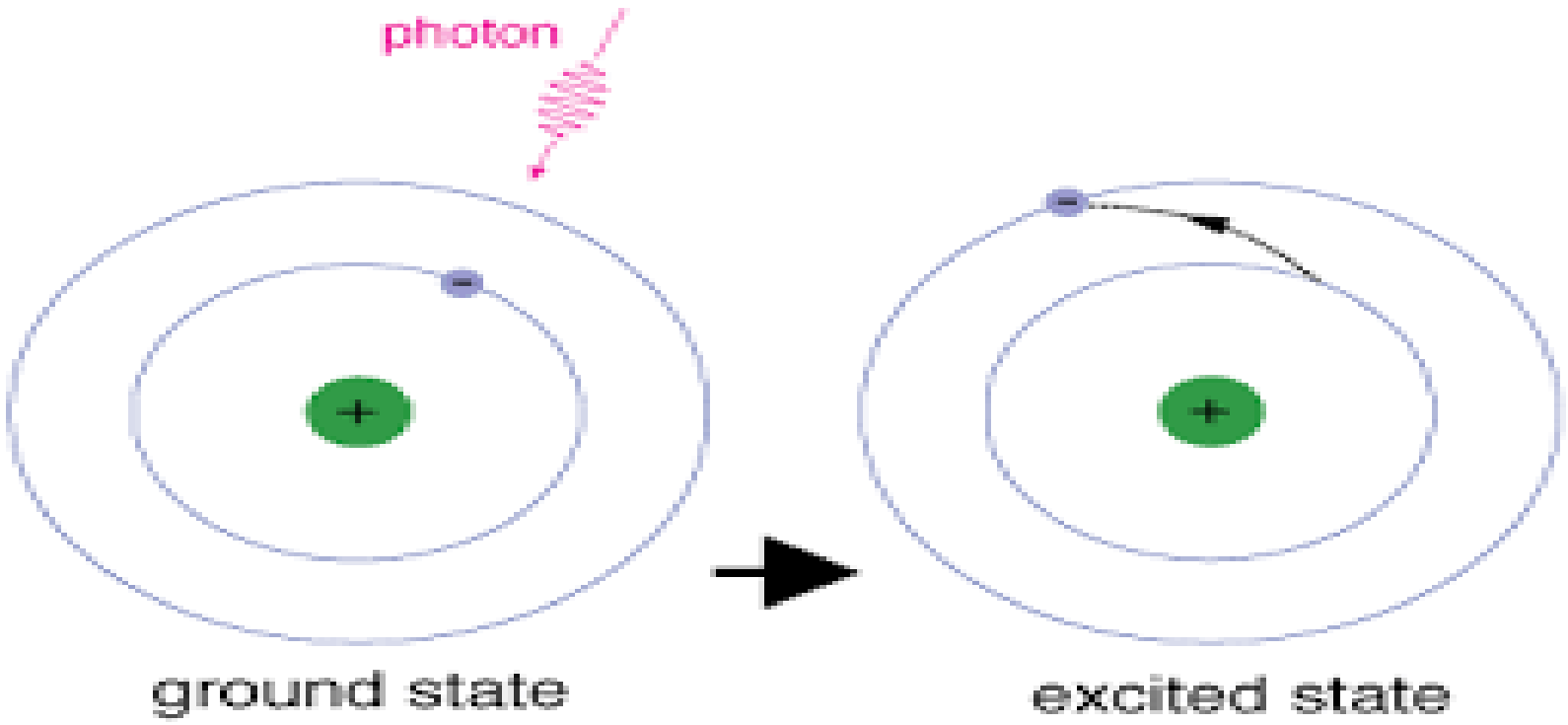
UN Sustainability Goals

Are a set of goals that aim to end poverty and protect the planet by 2030.

Chemistry and the atom



Energy Gap: Energy difference between the ground and excited state

Catalyst: A substance that increases the rate of a chemical reaction

PhotoCatalyst: a material that absorbs light to increase its energy level before transferring that energy to a responding substance to start a chemical reaction

Learn about Jack

Works as a quantum chemistry researcher in a company

Started his job this week

Specific focus of designing new catalysts for chemical reactions

1-2 % of annual energy on fertilizers production

Problem Statement

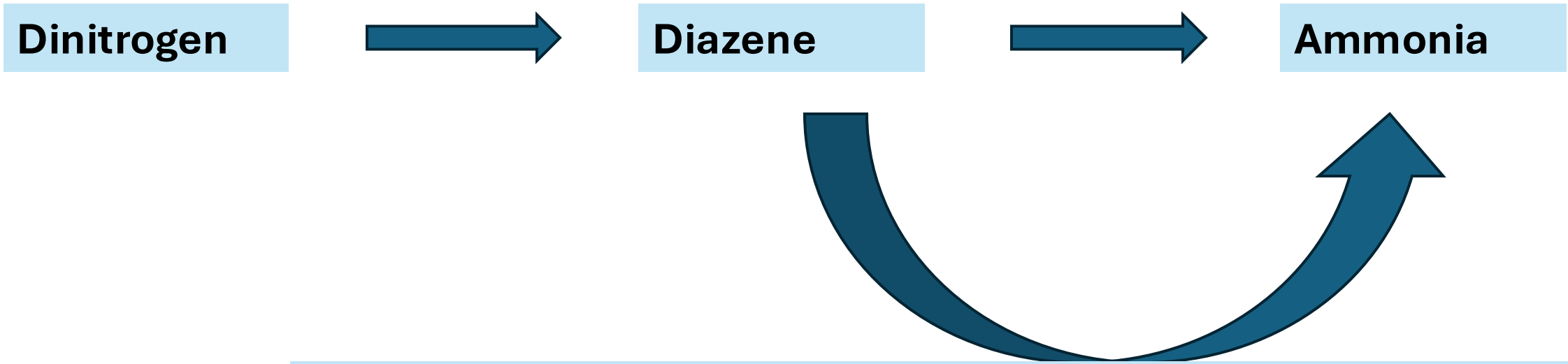
Dinitrogen

$$N_2 + 2H^+ + 2e^- \rightarrow N_2H_2$$

Diazene

$$N_2H_2 + 4H^+ + 4e^- \rightarrow 2NH_3$$

Ammonia



80% of annual Ammonia production is used in fertilizers
A Photocatalyst increases the rate and efficiency of this process

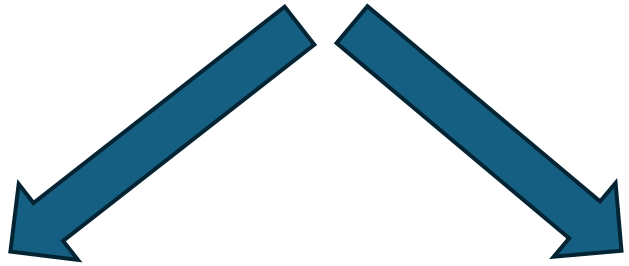
Relation to sustainability goals

More sustainable food production

Less emmition of CO2 due to more efficient reactions

Algorithms

Jack made his research and found two algorithms to try



SS-VQE

Subspace-Search VQE

Finds both ground and excited states using a variational circuit

QSE

Quantum Subspace Expansion

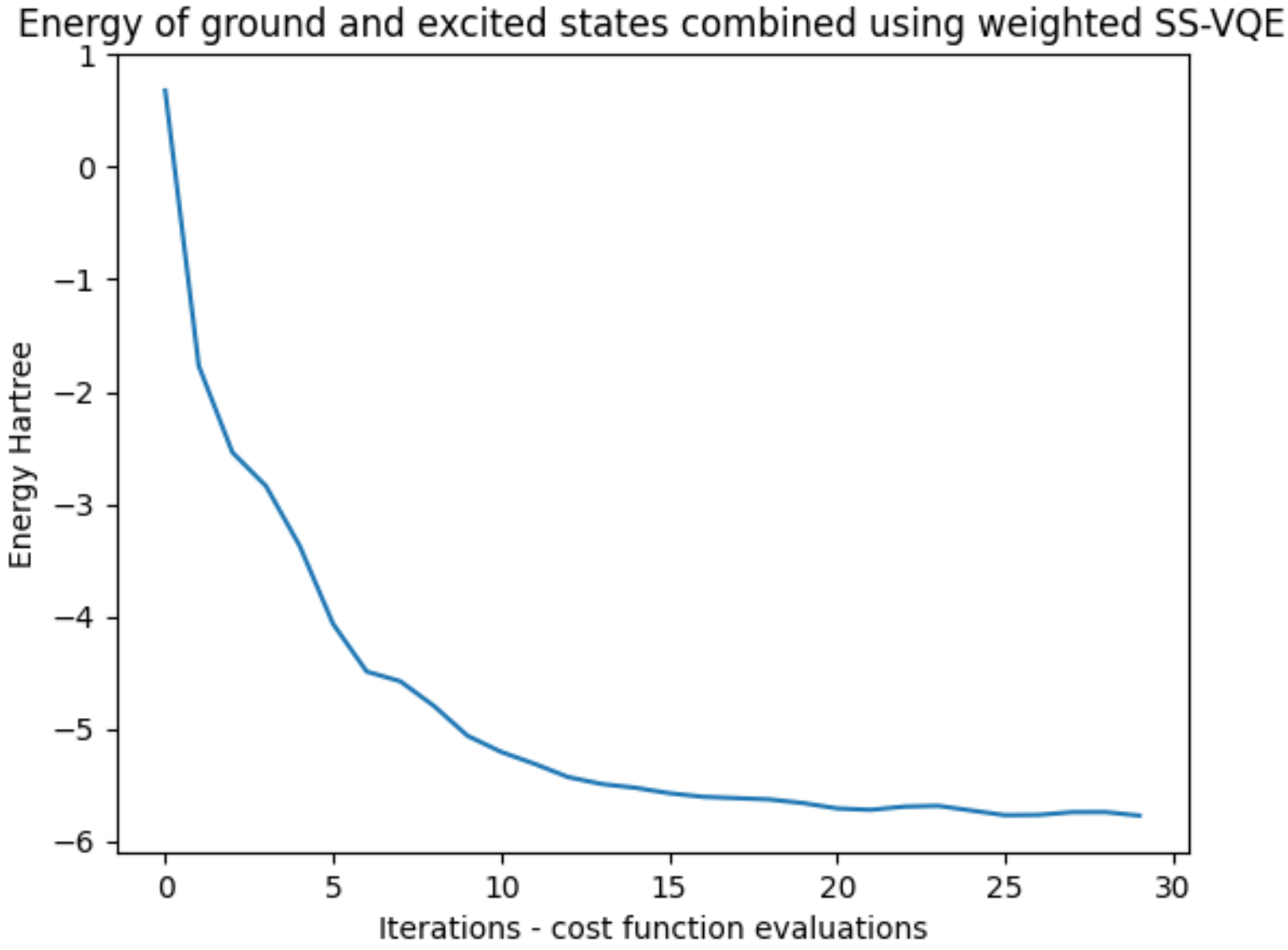
Finds the ground state energy using VQE then the excited after diagonalization

Results for H2

Algorithm	Ground E	1st excited E
SS-VQE	-1.12	-0.44
Pyscf	-1.03	-0.86

Algorithm	Ground E	1st excited E
QSE	-1.26	-0.824
Pyscf	-1.03	-0.86

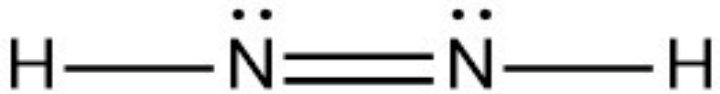
All energies are in Hartree



Results for N2H2 using QSE only

Requires 12 qubits to simulate → **Fix the first two orbitals** → **Requires 8 qubits to simulate**

Finding the gap energy between 1st excited and ground state is far more important than the exact energy for the photocatalyst



diazene

Algorithm	Ground vs 1st excited energy gap	Ground vs 2nd excited energy gap
QSE	0.102	0.166
Pyscf	0.117	0.163

Future directions

Accuracy was good but chemical reactions require higher accuracy

Access to HPC devices to run for complex molecules and more accuracy

Studying the effect of noise in noisy simulators and real hardware

Thank You