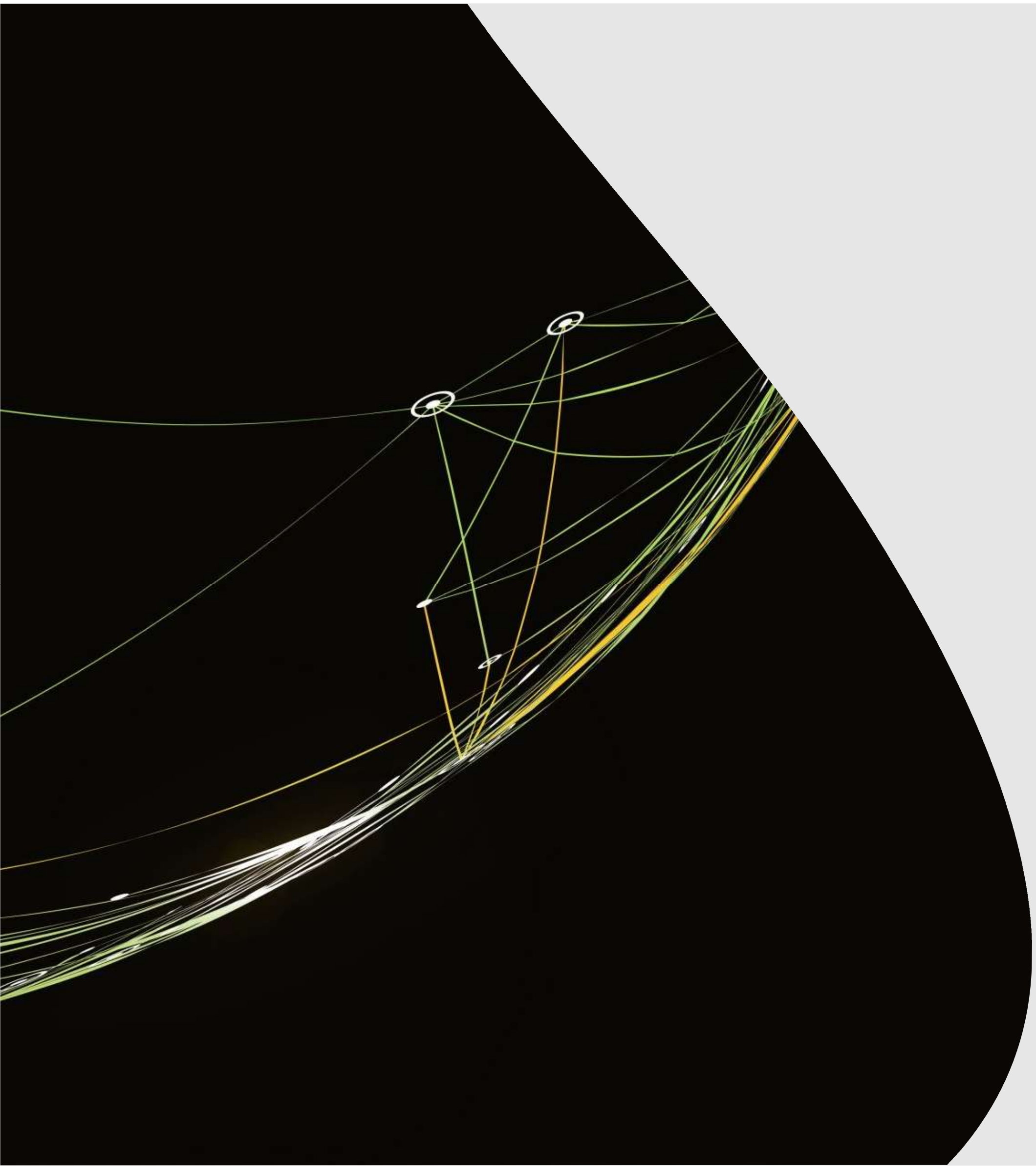


Technology in sustainability

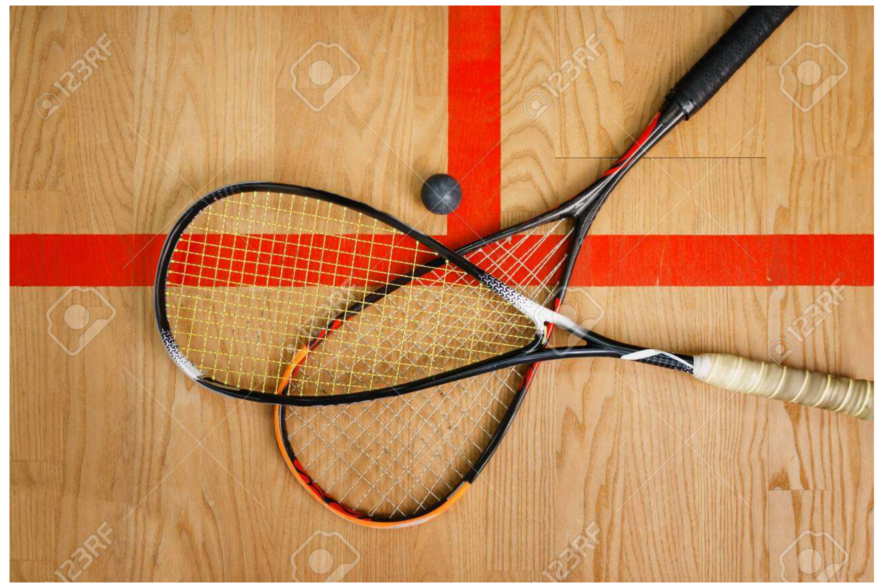
Hitarth Choubisa

Senior PhD student, Sargent Group

Electrical & Computer Engineering

About me:

- Final year PhD student in Sargent group @ECE
- Before pandemic, you could have easily found me in Galbriath Building
  - Now easier to find me on ZOOM
- When I am not burning some CPUs and GPUs, you can find me *playing squash* or watching Ghibli ☺

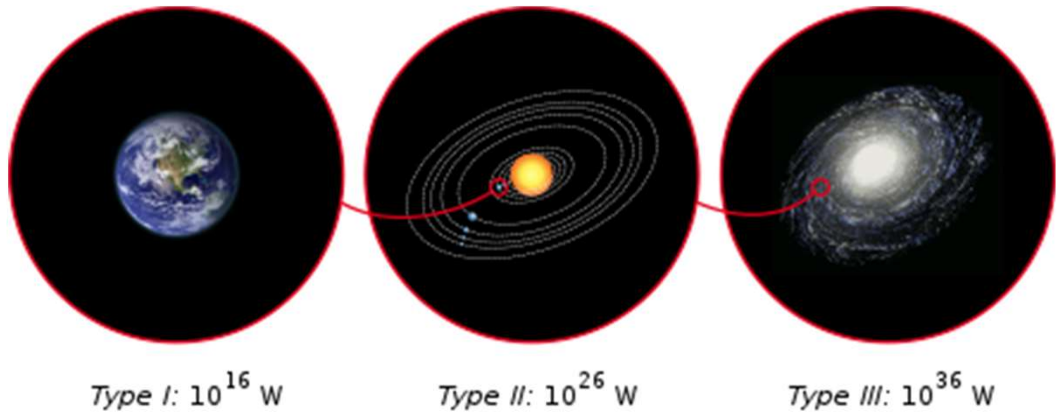


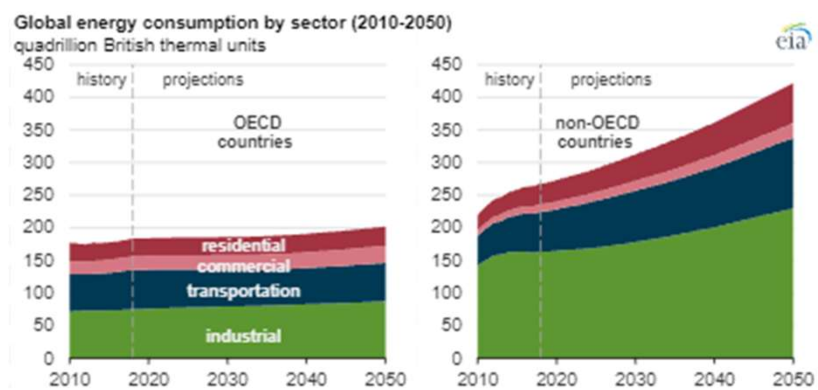
ENERGY:

- Energy consumption levels has been linked to technological advancements of a civilizations
  [Nikolai Kardashev, 1964]

- Kardashev proposed 3 categories of civilizations

- At least for now, energy demands have been projected to increase by 50% by 2050 ☺

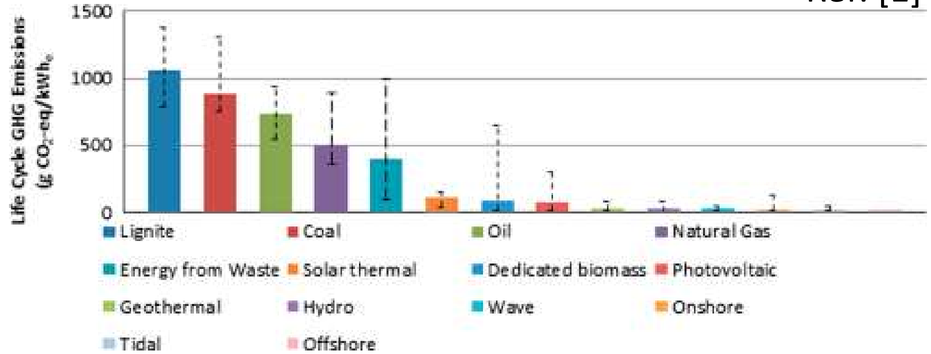




Source: EIA

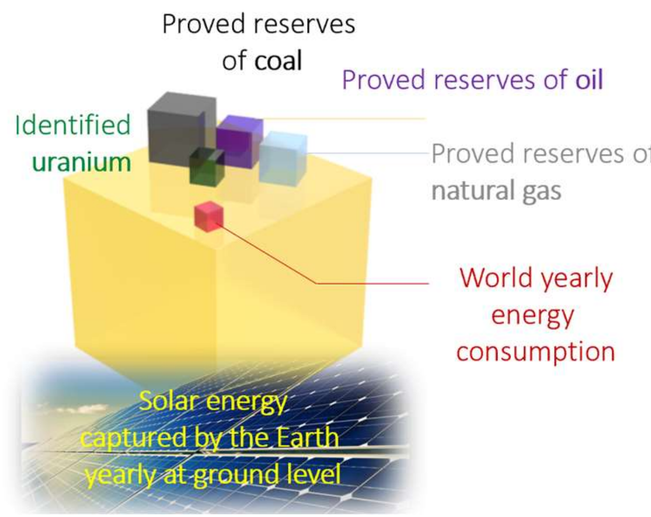
RENEWABLE ENERGY:

Ref: [1]



- How can we harness energy without breaking the nature i.e. sustainably?

- Renewable energy and renewable fuels!
  - Improvements in energy capture and energy storage



Abundant Renewable Energy

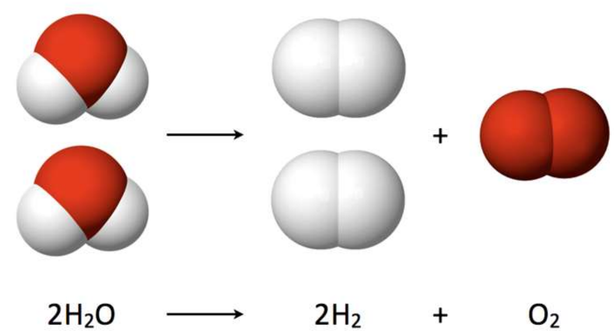
RENEWABLE ENERGY AND FUELS:

Energy capture:

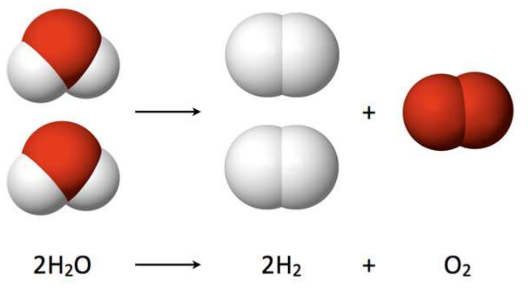
- *Solar cells*: Sun
- *Thermoelectrics*: Geothermal, heat sources, wasted heat
- *Piezoelectrics*: vibrational/mechanical sources
- *Renewable fuels*: reduction of CO_2

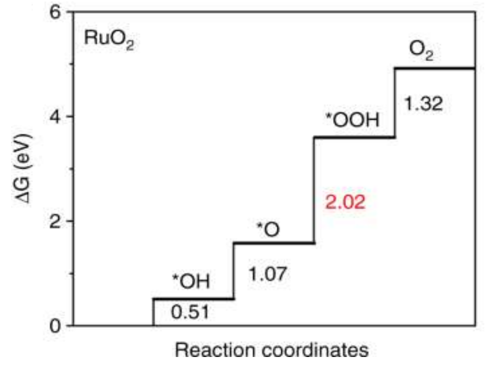
Energy storage:

- *Chemical based large scale energy storage*
  - *Comparison to Li-ion for large scale*
  - Water splitting: store water as H_2 and O_2
  - Alternatives to water: more valuable than O_2 and H_2 ☺
- *Battery materials*



A FEW EXAMPLE CHALLENGES:

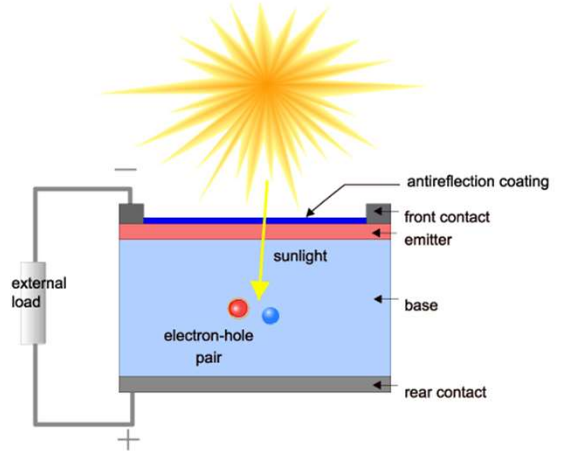




THERMODYNAMICALLY UNFAVORABLE

CORROSIVE ENVIRONMENT

EXPENSIVE CATALYSTS: Ir-based



SQ limit of single junction efficiency: 33%

Efficiency!

Defects!

Stability!

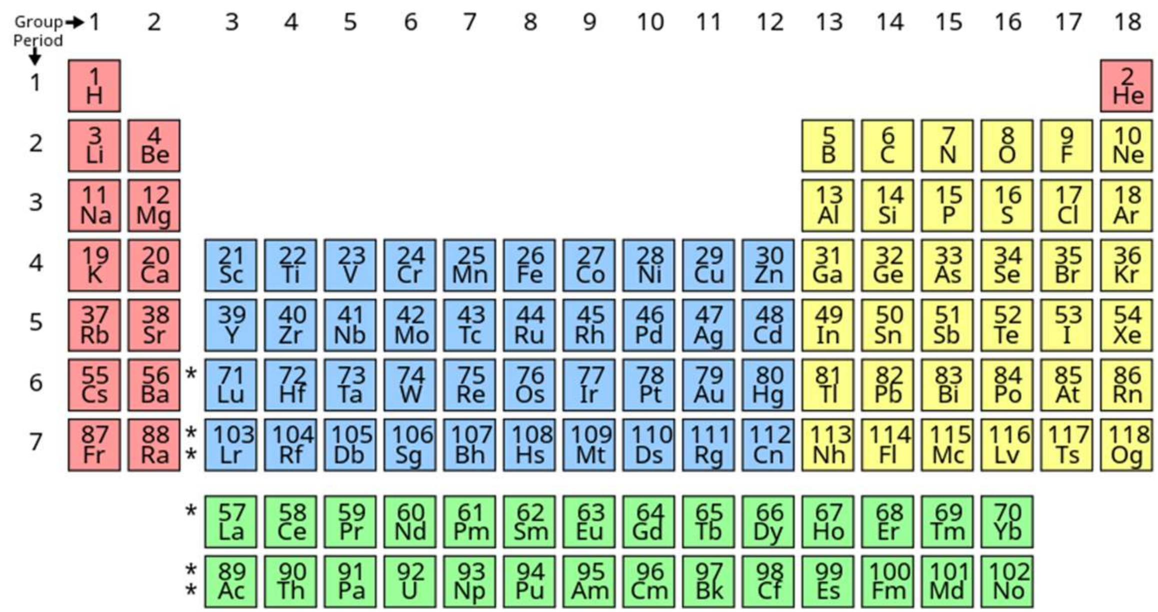
Scalability!

Environment friendly!

MAJOR CHALLENGES:

- Better materials and compounds!
  - More efficient
  - More stable
  - More earth-abundant*

- 118 elements – nearly “countless” possible combinations:
  - With 4% doping, using group theory we estimated, there are possibly 10^{18} compounds if we just have 8 elements at our hand in a single spacegroup!



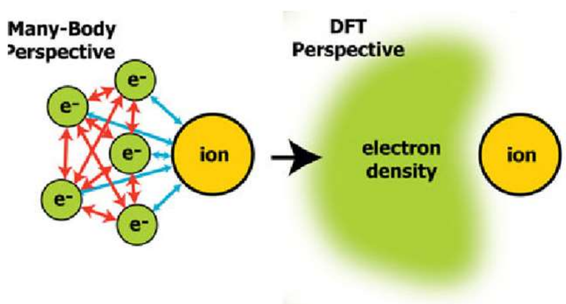
WHAT ARE THE SOLUTIONS? SOLUTION 1

Quantum mechanical simulations to predict our reality

Schrodinger's equation:

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \widehat{\boldsymbol{H}}|\Psi(t)\rangle$$

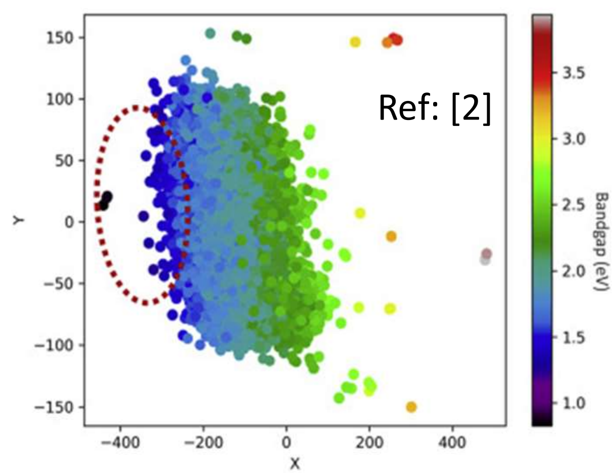
Density Functional Theory (DFT):



A single accurate DFT calculation takes > 2000 CPU hours. Cannot be used to scan materials space !! And what if you do not know the structure?

For single junction solar cells, we need materials with smaller bandgaps: this enables energy capture from wider range of wavelengths

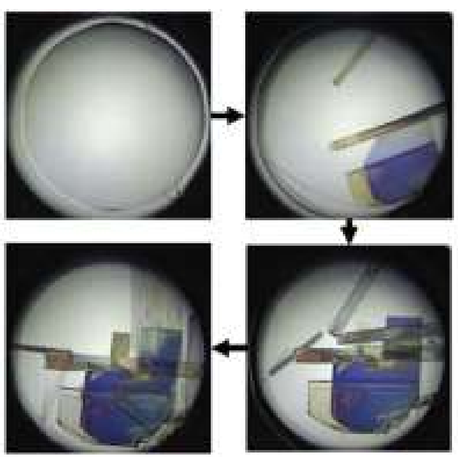
Autoencoder to the rescue!



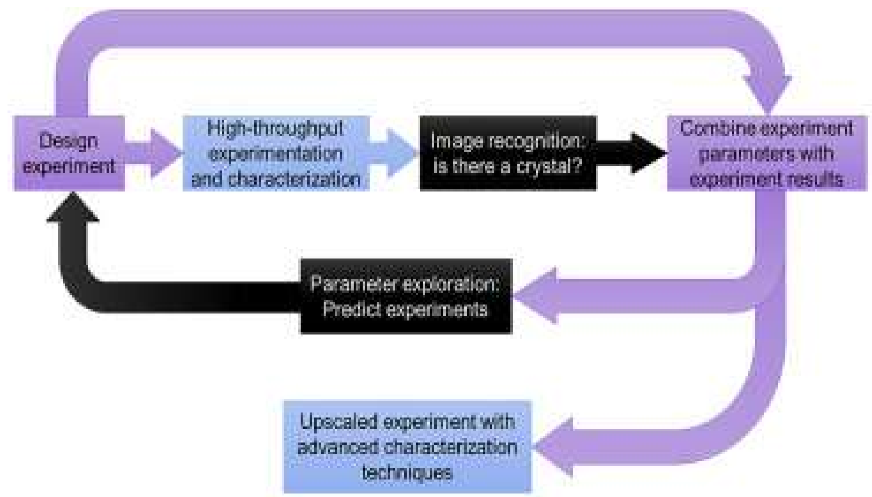
We predicted small amount of Cd doping can help bring the bandgap to the desirable numbers. Recently there has been experimental reports that support this! ☺

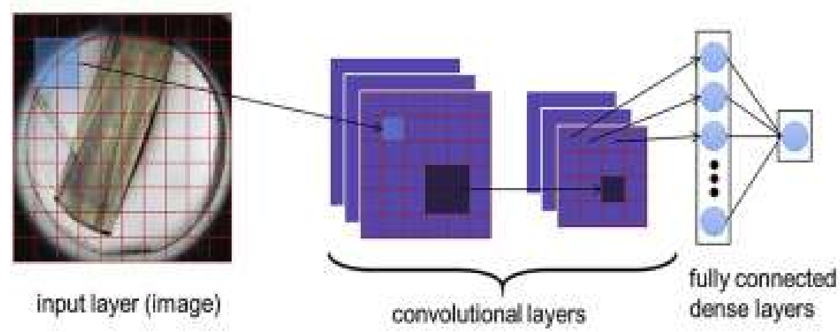
SOLUTION 2

- Robot driven high throughput experimentation
  - Robotic synthesis and characterization



3 hours lapse

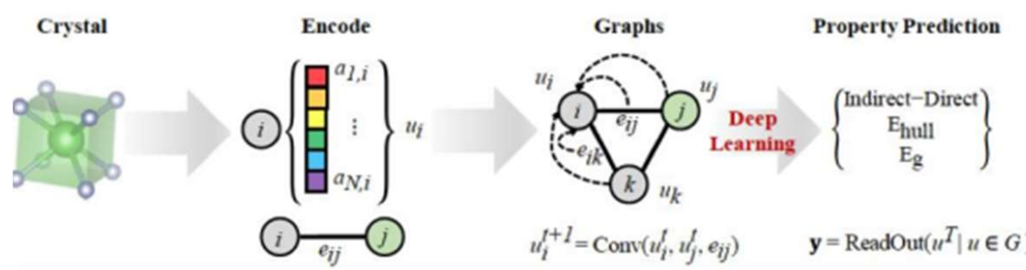


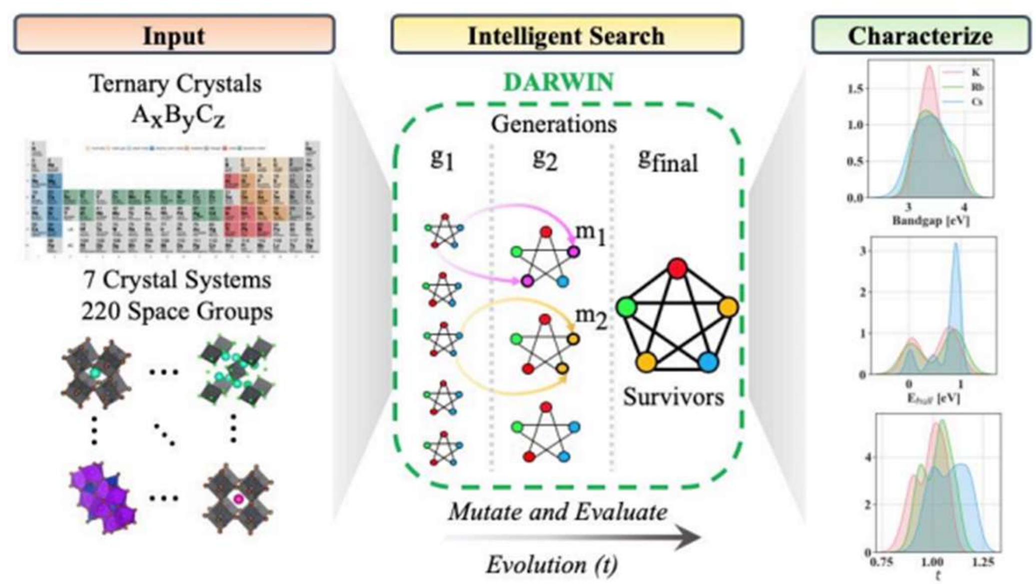


Ref: [3]

SOLUTION 3

- Extract scientific knowledge!
- Learn from trained machine learning models
  - Extract non-trivial physics and chemistry





Ref: [4]

WHAT DOES FUTURE HOLD?

Applying developed methods to develop new materials and **test them**!

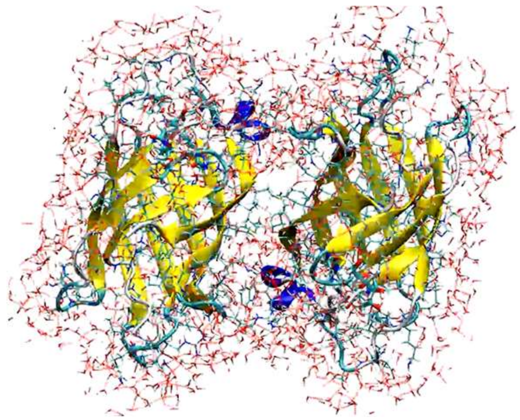
Develop better models of reality

- Universe is much more complex
- Simulate realistic systems:
  - Just 18 grams of water has $6.023 \cdot 10^{23}$ molecules
- Longest simulation ever being done: ~1 millisecond[5]
  - ~15000 atoms

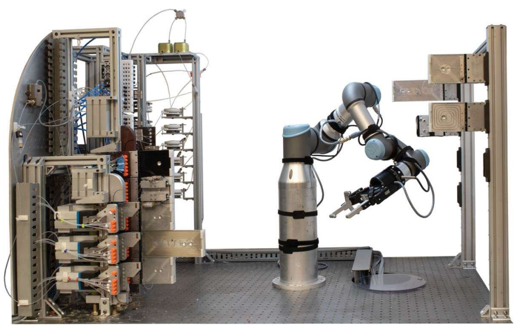
Develop methods to accelerate quantum chemistry and Machine Learning:

- Predict beyond type of data ML is trained on
- Theory driven robotic experiments
- Successful hits in minimum trials
- Quantum computing

ASE ANI: 40,000 atoms

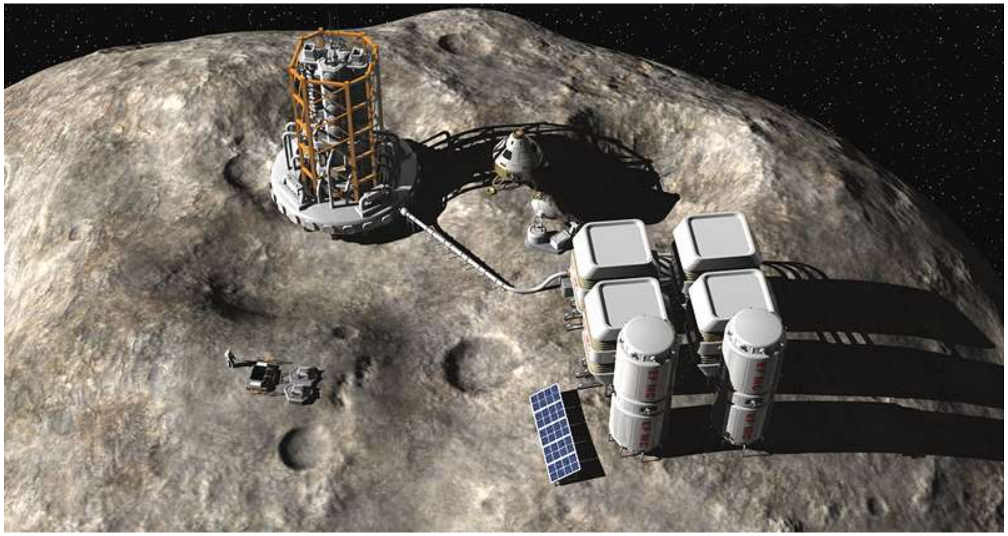


Robotic synthesizer



WHAT DOES FUTURE HOLD?

Space mining



END NOTE:

- We are always looking for students and researchers to come join us!
  Sargent Group, University of Toronto

- If you are interested in clean energy research, machine learning, quantum chemistry, chemistry, physics, machine learning, robotics, quantum computing, material science or public policy and want to learn by contributing – feel free to reach out anytime!
  - Some knowledge of Python will definitely help ☺

[*hitarth.choubisa@mail.utoronto.ca*]

Before covid!

References:

1. Renewable and Sustainable Energy Reviews 39 (2014): 461-475
2. Matter 3.2 (2020): 433-448
3. Matter 2.4 (2020): 938-947
4. arXiv preprint arXiv:2101.04383 (2021)
5. Science, 334(6055), 517-520.