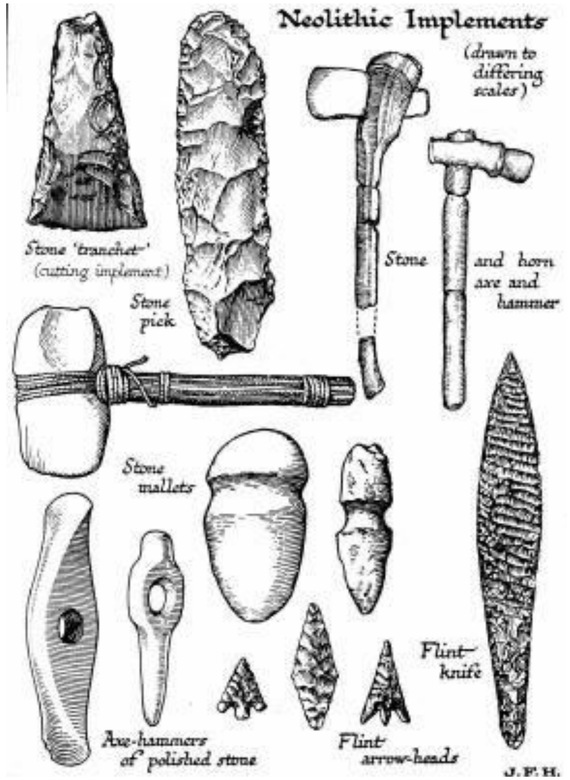
Material Informatics – Road Map for Future Material Discovery

Chirantan Gangully
MTech. Functional Materials and Devices
23PH63R06

Need for Material Discovery

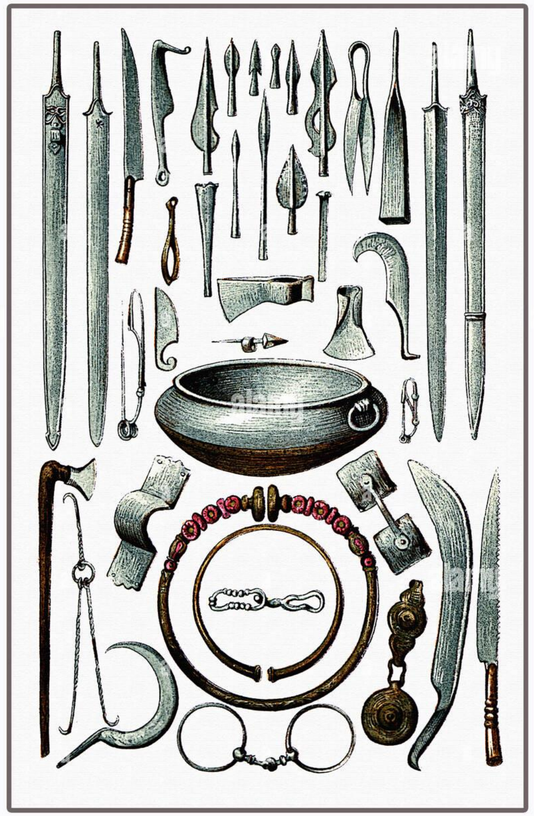
Essential for the progress of humanity!!

Stone Age



Bronze Age

Iron Age

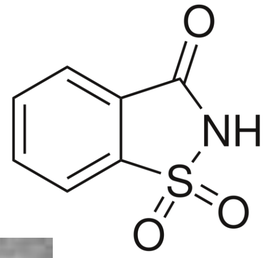


Semiconductor Age

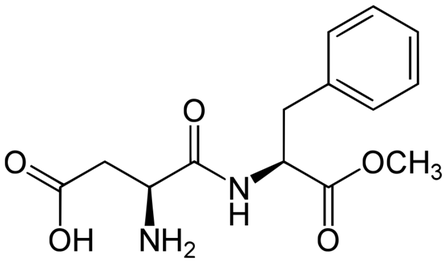
History of Material Discovery

Lucky accidents

Saccharin (Artificial Sweetener)

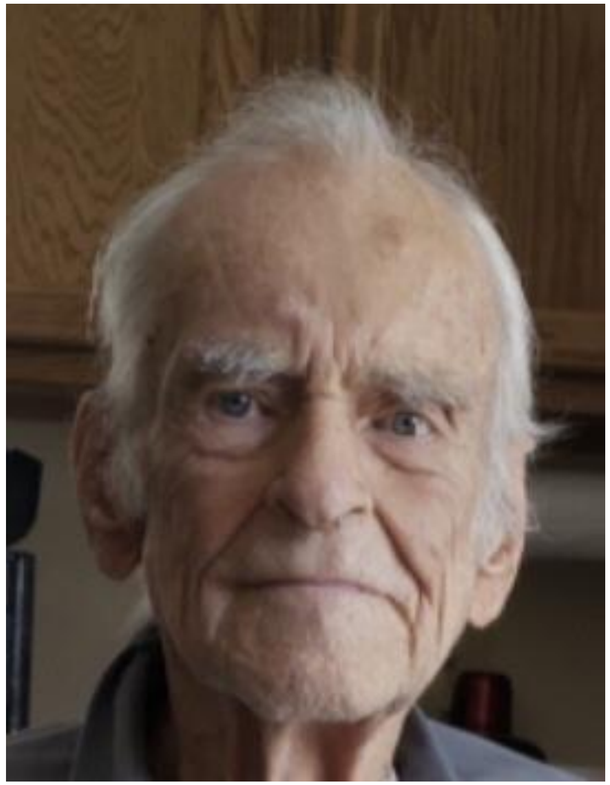


Aspartame (Artificial Sweetener)



Constantin Fahlberg (1878)

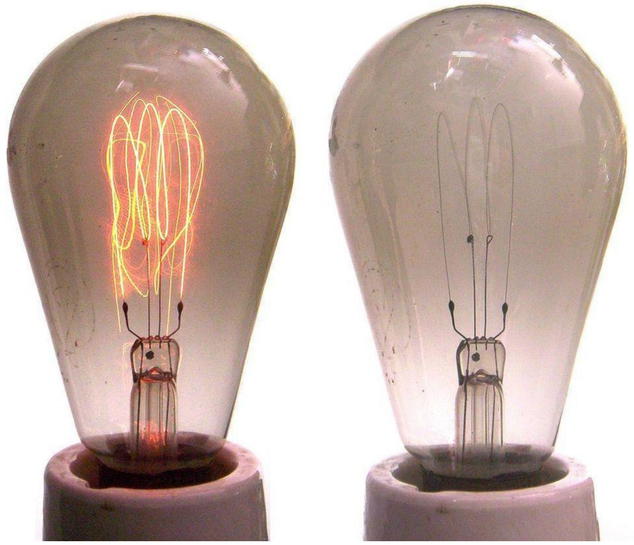
!!VERY UNSAFE!!

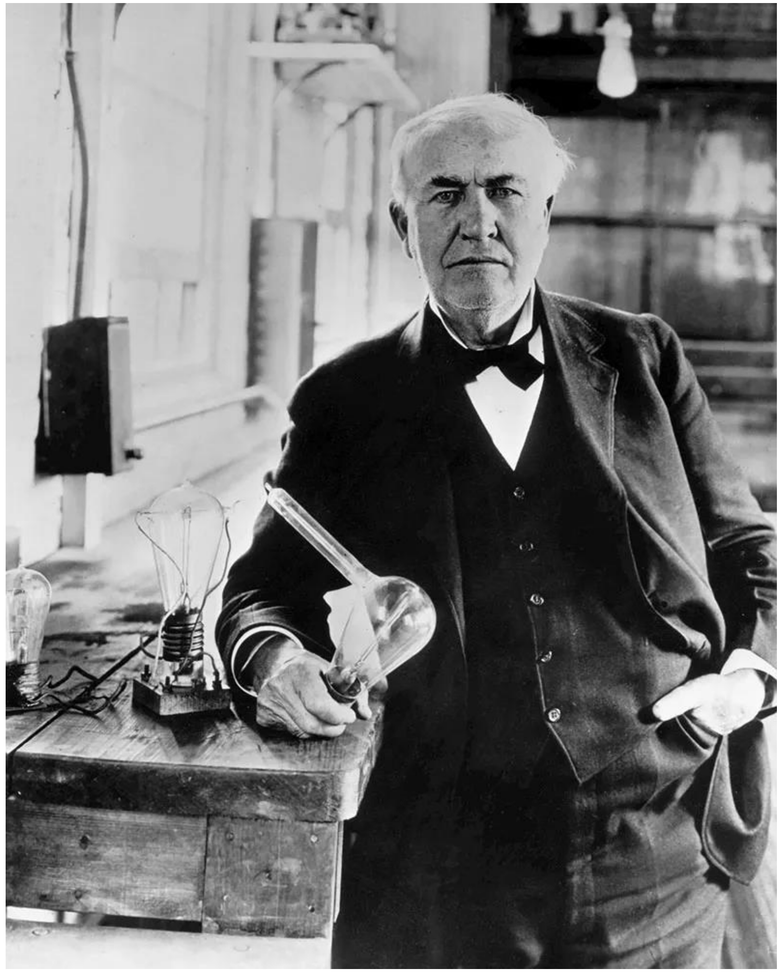


James Schlatter (1968)

History of Material Discovery

Trial and Error Method





2000+ Materials screened

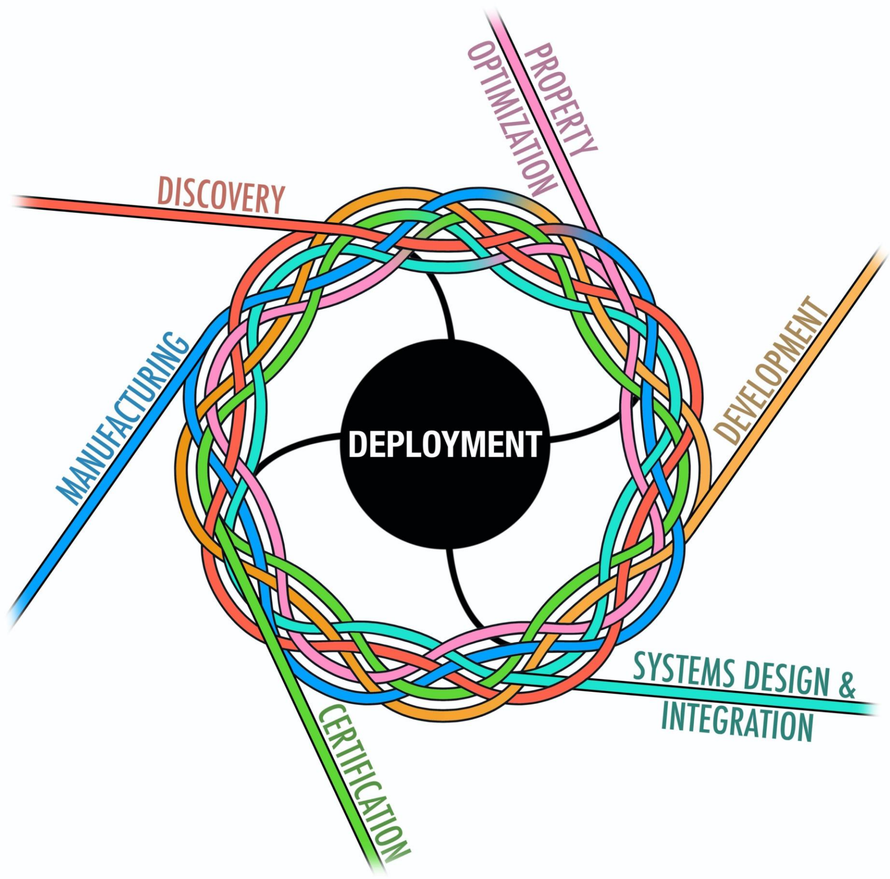
-Time and Resource heavy process

- Slow and gruelling process

!!NOT GOOD ENOUGH!!

Materials Genome Initiative

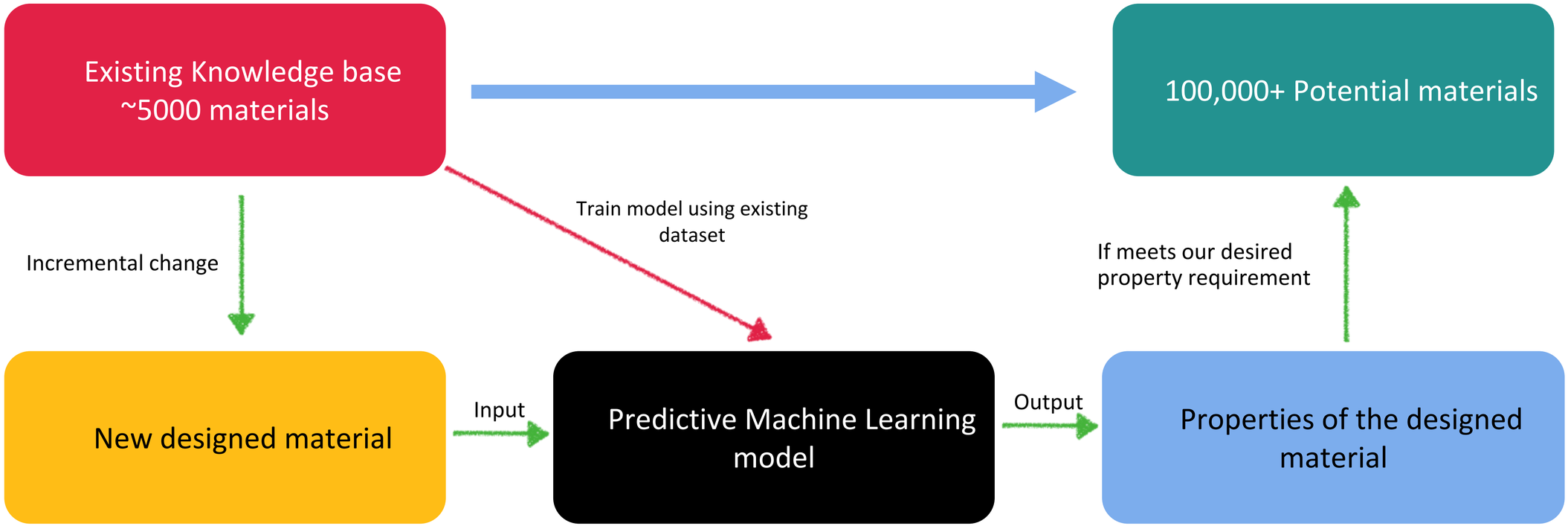
Goal: Discover - Deploy advanced materials twice as fast and at a fraction of cost



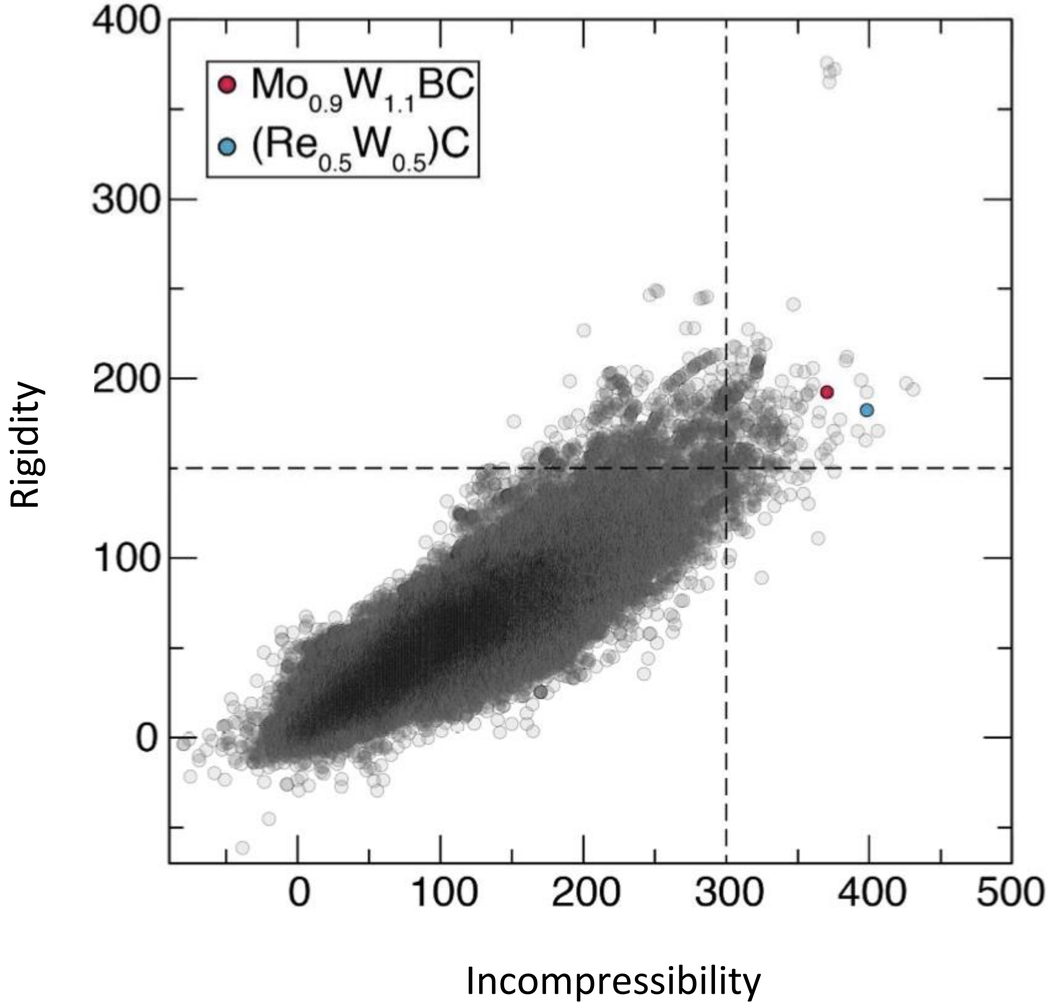
- A shift from physical design to simulation based approach.
- However, simulation of novel material properties is computationally intensive. (Can take weeks of time)
- A large database of known materials is created.
- Machine learning models are trained on these dataset to make predictions about novel materials in seconds.

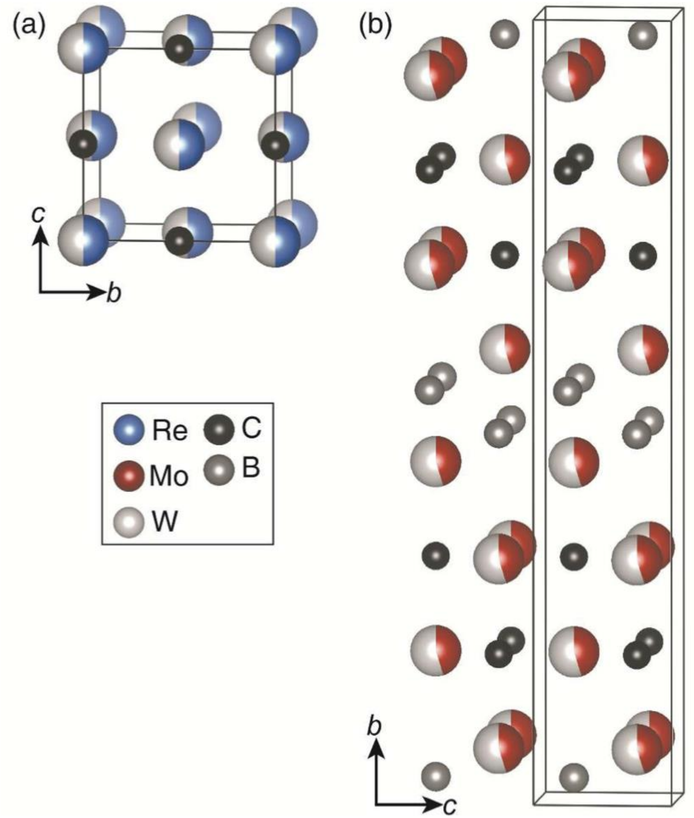
How can ML help?

Use case: Ultra Hard (cheap) materials for boring/drilling



ML aided search for superhard materials





Ref. Mansouri Tehrani, A., Oliynyk, A. O., Parry, M., Rizvi, Z., Couper, S., Lin, F., … Brgoch, J. (2018). Machine Learning Directed Search for Ultraincompressible, Superhard Materials. Journal of the American Chemical Society, 140(31), 9844-9853. doi:10.1021/jacs.8b02717

Some other discoveries

Some other critical materials has also been discovered using Materials Informatics

3D Printable Aluminium Alloy

Dye-Sensitized Solar Cell

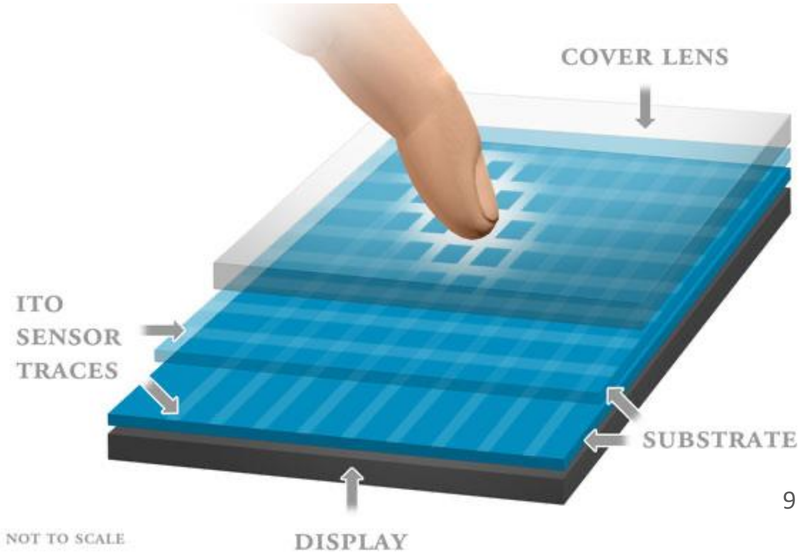
Some other discoveries

Some other critical materials has also been discovered using Materials Informatics

Transparent Conducting Oxides

Indium Tin Oxide - Transparent material that conducts electricity.

Applications:
1. Touch screen application
2. Reflects Radar waves (stealth fighters)



Transparent hard materials

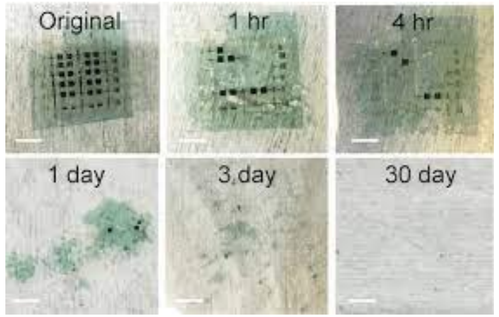
Aluminium oxynitride - hardest polycrystalline transparent ceramic available commercially.

Applications:
1. Blast-proof/bullet-proof windows

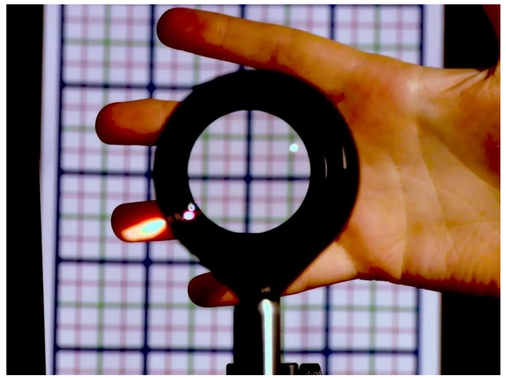
What’s the Future?

- **Indestructible fiber**

- **Completely Biodegradable Electronics**



- **Lightbending Invisible Meta-Materials**



!!Be creative, possibilities are infinite!!

Thank You