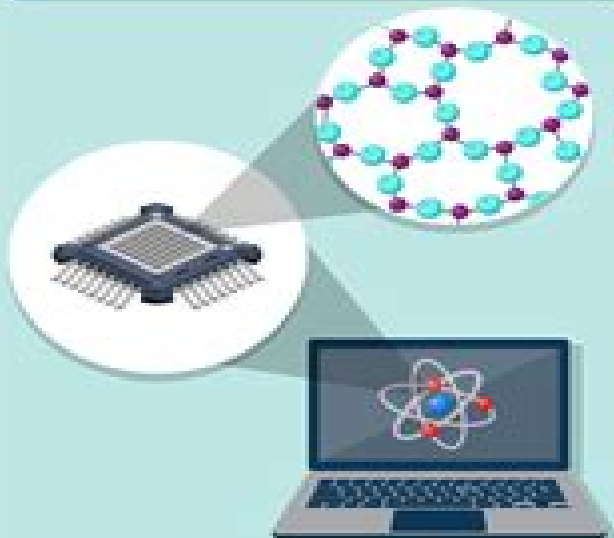


Using Artificial Intelligence for New Material Discovery

Materials
Advances



Amorphous alloys allow for lower deposition temperatures than crystalline materials, enabling complex transistor architecture



However, more techniques are needed to screen new materials' properties and gauge their practical suitability



Can artificial intelligence help screen new amorphous materials?

Calculated properties of simple binary amorphous structures based on known crystals



Trained machine learning (ML) models to predict properties of complex oxides



Optimized an objective function to find ideal candidates in the full chemical space and validated these results



The ML model could predict the properties of amorphous oxides

Elements considered:

12
Mg

13
Al

14
Si

22
Ti

30
Zn

31
Ga

40
Zr

47
Ag

48
Cd

49
In

50
Sn

51
Sb

Zn-Mg-Al-O alloy was identified as a promising candidate material

Advantages of using this approach:

✓ Fast training

✓ Stable predictions

✓ Easy to use

✓ Customizable training dataset

This pipeline can be used for any alloy/compound discovery problem

ML and *ab-initio* methods can be combined to calculate pivotal materials properties and identify suitable materials for various applications

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