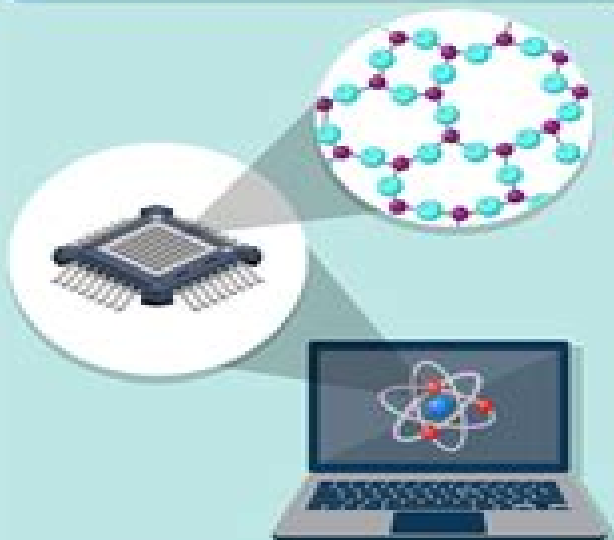


Using Artificial Intelligence for New Material Discovery

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

Making New Material

S Baum



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Table of Contents Making New Material

1. Understanding the eBook Making New Material
 - The Rise of Digital Reading Making New Material
 - Advantages of eBooks Over Traditional Books
2. Identifying Making New Material
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Making New Material
 - User-Friendly Interface
4. Exploring eBook Recommendations from Making New Material
 - Personalized Recommendations
 - Making New Material User Reviews and Ratings
 - Making New Material and Bestseller Lists
5. Accessing Making New Material Free and Paid eBooks
 - Making New Material Public Domain eBooks
 - Making New Material eBook Subscription Services
 - Making New Material Budget-Friendly Options

6. Navigating Making New Material eBook Formats
 - ePub, PDF, MOBI, and More
 - Making New Material Compatibility with Devices
 - Making New Material Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Making New Material
 - Highlighting and Note-Taking Making New Material
 - Interactive Elements Making New Material
8. Staying Engaged with Making New Material
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Making New Material
9. Balancing eBooks and Physical Books Making New Material
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Making New Material
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Making New Material
 - Setting Reading Goals Making New Material
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Making New Material
 - Fact-Checking eBook Content of Making New Material
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
 - Integration of Multimedia Elements

- Interactive and Gamified eBooks

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