Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

Materials Genoma

Computational materials discovery

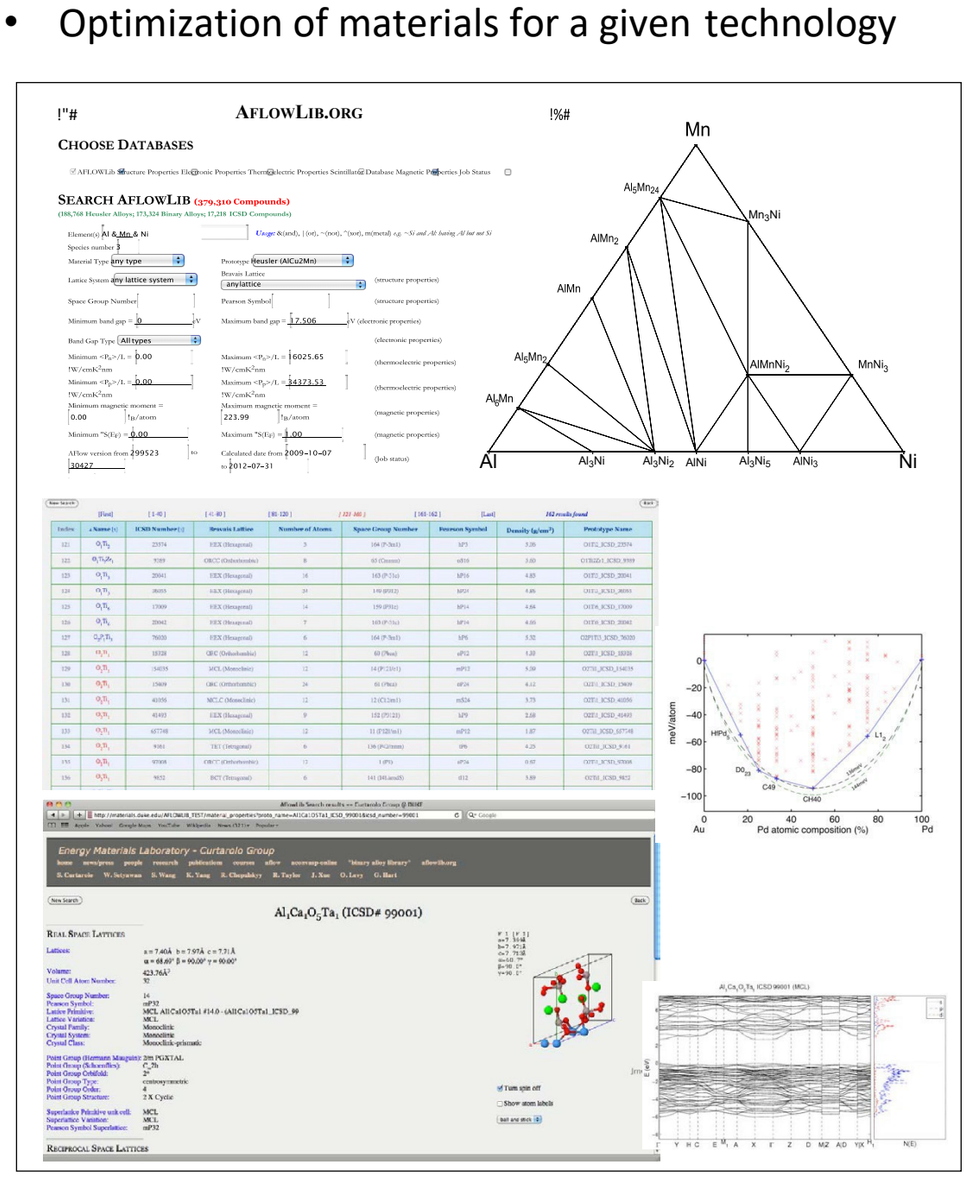
Overview

The Materials Genoma is a computational technology allowing the discovery of new materials phases (new compounds) optimized for specific applications. It is based on advanced electronic structure methods combined with contextual analysis, machine learning and large database creation.

What Problem does it Solve/Advantages

Standard materials discovery based on an entirely experimental approach is usually slow, costly and does not allow for radical breakthrough (it is largely incremental over existing materials). Materials Genoma allows us massive database search and high---throughput accelerated materials discovery. Some of the advantages are:

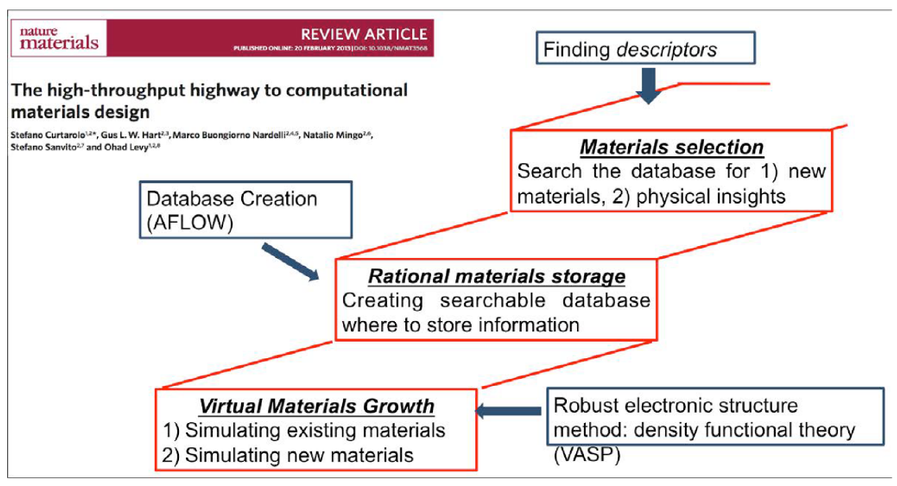
- Materials can be screened and evaluated at virtually no cost (feasibility assessment of materials)
- Large dataset is available
- Rapid screening and high---throughput discovery
- Multiple---parameter optimization can be performed
- Optimization of materials for a given technology



Possible Applications

Applications for this technology can be found in all sectors requiring novel materials phases:

1. Optimization of alloys for multiple applications
2. Novel magnets for energy
3. Novel magnets for data storage
4. Novel materials for batteries
5. Novel electronic materials
6. Novel thermoelectric materials



Technology and Patent Status

The method is based on density functional theory (VASP code) and an algorithm to create and store results in databases (AFLOW). AFLOW is developed by University of Duke (TCD Collaborator). The database is not publicly accessible, and its content is protected.

The opportunity

This technology is under continuous development, with a large database of >3.8 million compounds currently available.

Materials Genoma is suitable for companies seeking large materials screening and who are critically dependent on delivering new materials phases.

Our preferred mode of engagement is through collaborative projects. Please contact us if you are interested in research in this area. There are various support mechanisms and grants suitable for furthering or customizing the technology to a particular application.

https://doi.org/10.1016/j.commatsci.2012.02.002

Market

Processing Technology and Novel Materials

IP Status

Copyright

Opportunity

Research collaboration

Available to License

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