



# 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 artificial intelligence algorithms 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 are 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

