Classification of Half-Heusler Compounds Using A Machine Learning Approach

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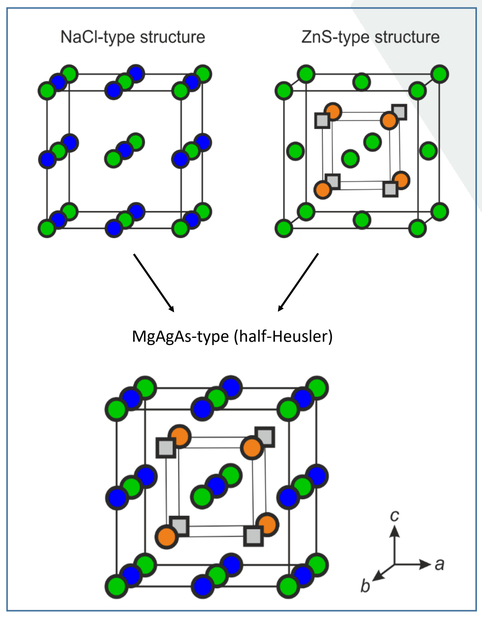
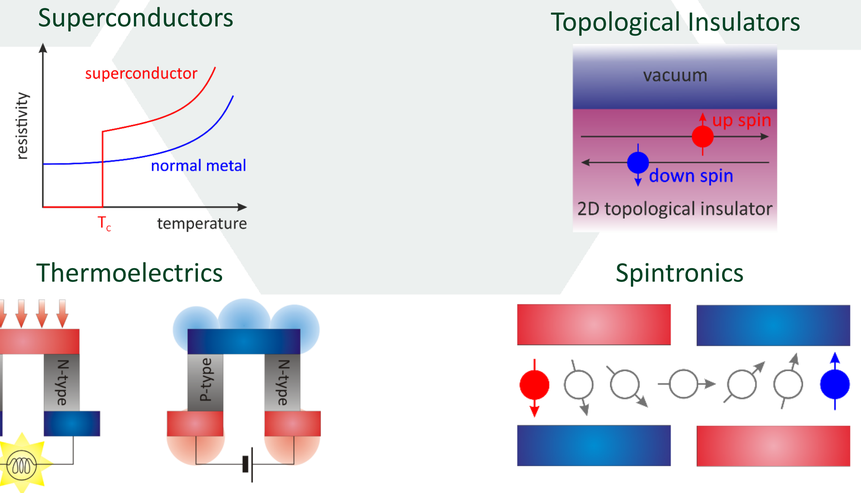
BACKGROUND

Half-Heusler compounds form a large versatile class of solids with cubic structures having many applications as thermoelectric materials, spintronic materials, superconductors, and topological insulators. Many half-Heusler compounds conform to a structural description that combines features of the more covalent zincblende-type (ZnS) and more ionic rocksalt-type (NaCl) structures. However, there are notable exceptions (such as MgAgAs, GdPtSb, and PdHoBi) that do not. We have applied machine-learning approaches(through a support vector machine model) to classify, verify, and predict half-Heusler compounds.



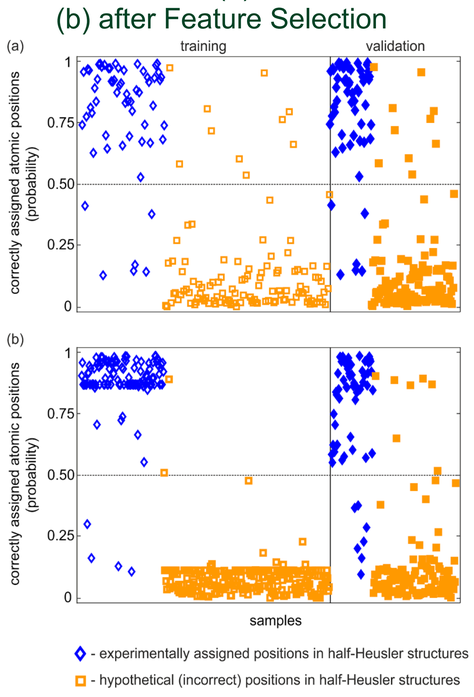
AIMS AND OBJECTIVES

The model is able to determine which element occupies tetrahedral vs. octahedral sites, distinguish between ternary compounds that half-Heusler and those that are not, and predict half-Heusler compounds. Proper classification is important to establish a structure-property relationship. Potential applications for half-Heusler compounds are listed below.



RESULTS

SVM Models (a) before and (b) after Feature Selection



Features

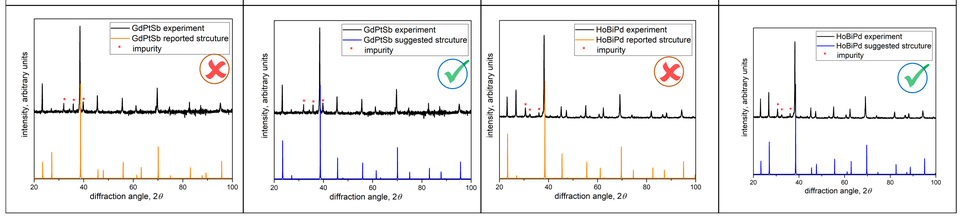
1. Atomic number
2. Atomic weight
3. Atomic radius
4. Covalent radius
5. Metallic radius
6. Single bond radius
7. Zunger radii sum
8. Ionic radius
9. Crystal radius
10. Pauling electronegativity
11. Martynov-Batsanov electronegativity
12. Gordy electronegativity
13. Mulliken electronegativity
14. Allred-Rochow electronegativity
15. Metallic valence
16. Number of valence electrons
17. Number of outer shell electrons
18. Thermal conductivity
19. Heat atomization
20. Polarizability
21. Gilmor # of valence electrons
22. Metal\Metalloid\nonmetal
23. Miracle radius
24. Mendeleev number
26. Period number
27. Group number
28. Family number
29. l quantum number
30. Melting point
31. Boiling point
32. Density
33. First ionization energy
34. Electrical conductivity
35. Specific heat
36. Heat of fusion
37. Heat of vapourization
38. Valence s
39. Valence p
40. Valence d
41. Valence f
42. Unfilled s
43. Unfilled p
44. Unfilled d
45. Unfilled f

Performance

	Before FS	After FS
MCC	0.798	0.900
Precision	0.871	0.925
F1	0.864	0.933
Error	0.089	0.966

The model can be used to perform data sanitizing

Element in position 4c (reported)	Element in position 4c (ML Suggested)	Element in position 4c (reported)	Element in position 4c (ML Suggested)
Sb(8.7% probability)	Pt(90.5% probability)	Bi(4.9% probability)	Pd(92.5% probability)

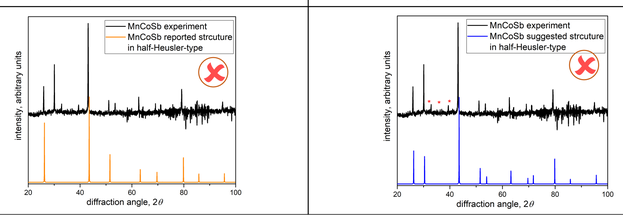


Also, the model can highlight structurally ambiguous compounds

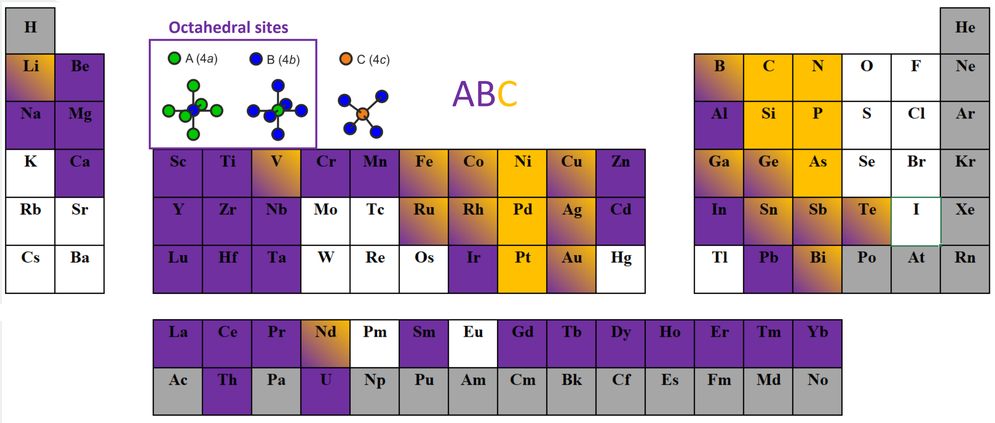
Compound	Element in position 4c (reported)	Element in position 4c (ML Suggested)
MnCoSb	Sb(32% probability)	Co(74% probability)

Single crystal diffraction data suggests the structure different from half-Heusler:

MnCoSb-type, known as 2x2x2 half-Heusler

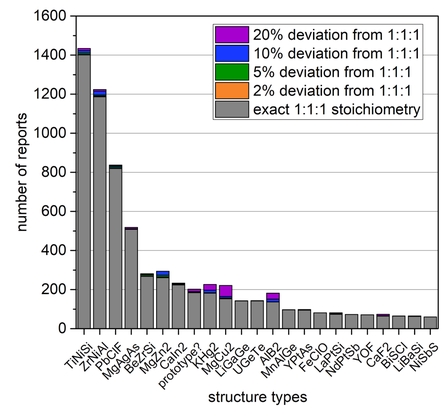


FUTURE DIRECTIONS



The model can successfully predict which site (Octahedral vs Tetrahedral) an element would prefer to occupy. We can then apply this to other systems with similar problems concerning site occupancy.

Determination of the correct structure will accelerate discovery of novel thermoelectric, spintronic and superconducting materials.



FES PROJECT OVERVIEW

T12-P01 "High-throughput materials discovery through materials genomics"

Discovering better materials is essential for tackling the enormous challenges in developing new renewable energy sources. The experimental variables that must be considered to optimize a given property are too many and their relationships are too complex to allow anything but incremental improvements to be made. So how do we think "outside the box" to find entirely new materials? As part of the larger effort known as the "Materials Genome Initiative," approaches based on data-mining and materials informatics techniques can help screen new compounds with desired properties and features, at greatly accelerated rates, and provide insights into the design principles required to engineer improved materials. These tools will be used, in particular, to find better photovoltaics and catalysts for solar fuels.

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FUTURE ENERGY SYSTEMS

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