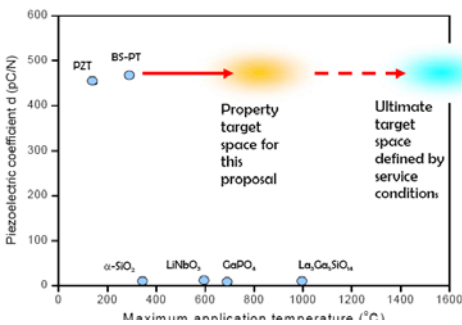


Discovery of High Temperature Piezoelectric Materials K. Rajan, Iowa State

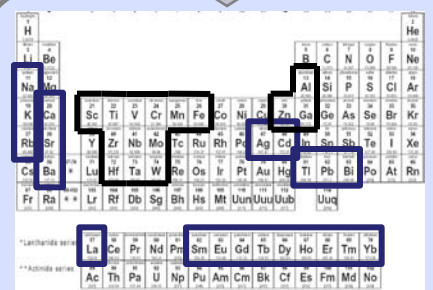
Combinatorial and High Throughput Discovery of High Temperature Piezoelectric Ceramics

STATUS QUO



Potential search space for very high temperatures (i.e., the oxides) have very low piezoelectric coefficients. Presently known ferroelectrics are not stable at high temperatures. Need a new materials discovery strategy

NEW INSIGHTS



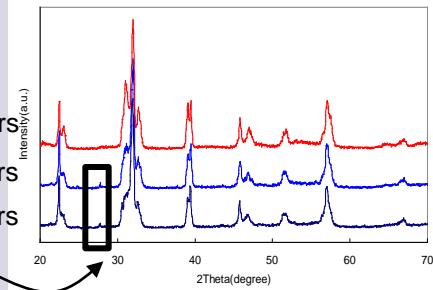
Establishment of combinatorial search space for complex oxides (eg. ABO_3) targeting perovskite structures & low tolerance factor

Establishment of coupled experimental and informatics based search strategy

MAIN ACHIEVEMENTS:

A. Synthesized single phase materials: critical for experimental studies

Single phase $0.65BiFeO_3-0.35PbTiO_3$ when calcination is 900C



2nd phase peaks

B Established new ABO_3 piezoelectric/ferroelectric database and discovered correlations between site chemistry and properties via data mining :

20 compounds- 45 crystallographic and electronic descriptors: including piezoelectrics and ferroelectrics

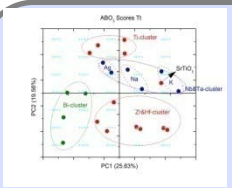
HOW IT WORKS:

- A. Systematic calcination studies to produce tetragonal phase
- B. Systematic literature and computational development of descriptors

ASSUMPTIONS AND LIMITATIONS:

- A. Control of purity and second phase formation during processing
- B. Disparate and sparse data in literature

QUANTITATIVE IMPACT



Data Mining

Ti contributes positively towards an increase in the transition temperature (T_t)

In $A^{1+}B^{5+}$ the impact of Nb and Ta on T_t are identical. So, the major difference in the property comes in from the A-site.

In $A^{3+}B^{3+}$, Bi-ion dominates the impact on T_t

END-OF-PHASE GOAL

End goal:

Discover new high temperature piezoelectric ceramics and establish informatics as a reliable tool for materials discovery :

Discovery of new high temperature piezoelectric materials and high throughput methodology for materials discovery

3 Key Questions

- *What are you trying to accomplish? Why?*
 - Discover new and still unexplored chemistries of high temperature piezoelectric materials
 - Need for materials to withstand temperatures as high as 1600C
- *How is it done today and what are the limitations?*
 - Present approach is purely empirical or Edisonian whether through experiments or computation. The results are either too slow or depend upon promising but unexpected results.
 - *What is truly new in your approach that will remove current limitations and improve performance?*
 - Use of novel combinatorial experiments to produce **bulk** materials
 - Application of informatics to both drive and analyze experimental studies
 - *By how much?*
 - Our approach can increase the search space by a factor of 100 or more and hence increase the chances of discovery

3 Key Questions

- *If successful, what difference will it make and to whom?*
 - Advance the development of devices and sensors in high temperature environments
 - *Is this fundamental research?*
 - Yes
 - *What areas of science does this impact?*
 - Materials science of chemically complex materials
- *Will this research change the “future”?*
 - Yes. This will establish a generic tool that will enable accelerated discovery, design and insertion of materials