Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Information-Driven Exploration of Crystal Chemistries for Radiation Detection Materials[1] KIM FERRIS, BOBBIE-JO WEBB-ROBERTSON, Pacific Northwest National Laboratory, DUMONT JONES, Proximate Technologies, LLC. — The ability to suggest promising materials and a priori eliminate unfruitful inquiry is the key to new crystal chemistry searches. Variable spaces tend to be large and poorly defined, and property measurements (and computations) of candidate materials are not abundant. For simple binary systems, the presence of structural polymorphs and higher order compositions for A(m)B(n); m,n=1-3 would combinatorially generate over 300,000 candidates, greatly complicating our ability to explore candidate spaces. We have used knowledge extraction methods to evolve structural signatures to direct searches using performance-based criteria. The exploratory data methods used both supervised (support-vector machines) and unsupervised (disorder-reduction and principal-component) classification methods for structural signature development. The development of new candidates for radiation detection materials will be used as the case example for this talk.

[1]The authors acknowledge support from the PNNL Laboratory- Directed Research and Development Program.

Gregory Exarhos
Pacific Northwest National Laboratory

Date submitted: 20 Nov 2006 Electronic form version 1.4