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Final Report: $LiCaAlF_6$:Eu Scintillator Family Neutron Detection

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$LiCaAlF_6$:Eu Scintillator Family Neutron Detection

PROJECT NUMBER: **OR12-LICAF-PD2Jf**

1. INTRODUCTION

This final report was prepared in accord with the following guidance provided by the sponsor.

1. **How the work was done, details of analysis methods, and discussion of problems and solutions**

The progress of work in this project, the details of the analysis methods, and discussion of problems and solutions is contained in the following documents which have been provided to DOE/NNSA/NA-22 via their WebPMIS project management system:

Deliverables:

- *Task 1.1 Report*
- *Task 1.3 Report*
- *Task 1.5 Report*
- *FY13 Annual Report*
- *Task 3.1 Report*
- *Tasks 3.2-3.4 Report*

Publications:

- Mao-Hua Du; David J. Singh; "First-principles study of electronic structure, defects, and activators in $LiCaAlF_6$". Proc. SPIE 8852, Hard X-Ray, Gamma-Ray, and Neutron Detector Physics XV, 885205 (September 26, 2013); doi:10.1117/12.2022864.

Presentation: at NA-22 *2012 - 2014* Program Reviews

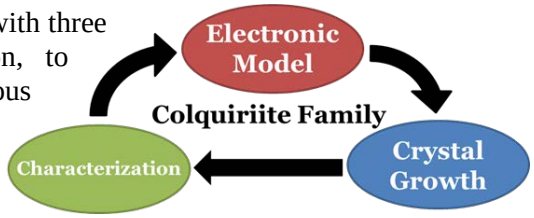
Project Documents:

- Final Project Life Cycle Plan

Quarterly Reports: each quarter from FY12 Q1 through FY15 Q2

2. **Retrospective view of the work, analysis, and problems/solutions at the end of the project**

The proposed work was based on a learning cycle format with three parts, (1) Modeling, (2) Growth, (3) Characterization, to investigate the family of colquiriite scintillators and various activating dopants as efficiently and effectively as possible. Under this research methodology, each of these functions would feed information to the next. Each



iteration around the cycle was expected to improve results and provide clues to the best path forward for the next iteration. However, it was realized that this research model is not robust and unable to handle setbacks at any one of the functions. Unfortunately, the project suffered setbacks in the "Growth" function and progress in the other functions was severely restricted. Of course, numerous alternative paths were trialed within the growth function to enable progress, but these required addition time and resources which in the end only provided limited progress. After reviewing the project as a whole, it can be concluded that the research model used was indeed too fragile for this sort of research and a more robust plan should be utilized in the future.

As a whole though, significant progress was made toward understanding the barriers toward realizing the benefits of this family of scintillators through modeling. Various paths forward were postulated, but limited growth and synthesis capabilities prevented experimental validation. Experimentally, it was found that the synthesis and growth of colquiriite scintillators requires special considerations for its thermodynamic and chemical properties. These were overcome in the end and a new, lower cost growth method realized, but too late to have a significant impact in validating modeling hypotheses.