

# **Molecular Foundry Conference and Abstract Call**

## **Report of Contributions**

Contribution ID: 0  
**Two-Dimensional Matter**

Type: **Symposium - Making, Measuring and Manipulating**

## Preparing AX2 compounds in a dry glove box.

PbCl<sub>2</sub>, SnCl<sub>2</sub>, BaCl<sub>2</sub> and BaI<sub>2</sub> all fall into a category of crystals known as AX<sub>2</sub> compounds. At ambient pressure, these materials are analogue compounds that crystallize at ambient conditions in the cotunnite (orthorhombic, Pnam) structure. The next phase (post-cotunnite (monoclinic, P1121/a)) is claimed to be the final step in the structural sequence for AX<sub>2</sub> compounds by Leger et al [1]. This holds significance because these compounds are iso-structural with a high pressure phase of silica, which is believed to be the primary component of rocky exoplanets.

**Primary author:** Mr SOUSTIN, Dmitry (LBNL)

**Presenter:** Mr SOUSTIN, Dmitry (LBNL)

Contribution ID: 1

Type: **Plenary session**

## Test abstract from Alison

We present the results of ab initio density functional calculations of perovskite-structure  $\text{La}(\text{Al,Fe,Cr})\text{O}_3$ . Our calculations reveal two structurally distorted ground states of opposite polarization. Motivated by the growth of three-layer superlattices with enhanced polarization, we investigate the ferroelectricity and magnetic ordering of the  $\text{La}(\text{Al,Fe,Cr})\text{O}_3$  system with the goal of finding emergent multiferroicity due to interfacial strain and inversion symmetry breaking. Finally, we investigate constrained tetragonal  $\text{LaAlO}_3$  to determine its role in the ferroelectric properties of the supercell.

**Primary author:** Dr HATT, Alison (LBNL)

**Co-author:** Dr COATES, Nelson (Cal Maritime)

**Track Classification:** Tract 1 (default)

Contribution ID: 2

Type: **not specified**

## Bio Symposia

*Thursday, 21 April 2016 09:00 (1 hour)*

Contribution ID: 3 Type: **Symposia - Product-Driven Research at the Molecular Foundry**

## This is a test title

This is a test abstract. I really like that markdown and latex is accepted in this interface as text boxes alone are really annoying.

Maybe add some instructions if were going to have a drop down menu for the type of submission.

**Primary author:** ALLEN, Corinne

**Presenter:** ALLEN, Corinne

Contribution ID: 4

Type: **Poster session**

## Test

Test

**Primary author:** TOMA, Francesca

**Presenter:** TOMA, Francesca

Contribution ID: 5  
**Materials**

Type: **Symposia - Structural and Functional Diversity in Porous Soft**

## Web Interface Trial

Blah blah blah

**Primary author:** Ms ARAMTHANAPON, Kristen (Sylvatex Inc.)

**Presenter:** Ms ARAMTHANAPON, Kristen (Sylvatex Inc.)

Contribution ID: 6

Type: **Plenary session**

**test**

test

**Primary author:** JOHNSON, Derrick (LBNL)

**Track Classification:** Tract 1 (default)



Contribution ID: 7

Type: **Plenary session**

## Personal email abstract apr 29

test

**Primary author:** Mr LEE, donald (lbnl)

**Track Classification:** Tract 1 (default)

Contribution ID: 8

Type: **Plenary session**

## personal abstract #2

test

**Primary author:** Mr LEE, donald (lbnl)

**Track Classification:** Tract 1 (default)