

# **Molecular Foundry Conference and Abstract Call**

Monday 18 April 2016 - Wednesday 18 May 2016

Molecular Foundry

## **Book of Abstracts**



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## Preparing AX<sub>2</sub> compounds in a dry glove box.

**Author:** Dmitry Soustin<sup>1</sup>

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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.

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## Test abstract from Alison

**Author:** Alison Hatt<sup>1</sup>

**Co-author:** Nelson Coates<sup>2</sup>

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We present the results of ab initio density functional calculations of perovskite-structure La(Al,Fe,Cr)O<sub>3</sub>. 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 La(Al,Fe,Cr)O<sub>3</sub> system with the goal of finding emergent multiferroicity due to interfacial strain and inversion symmetry breaking. Finally, we investigate constrained tetragonal LaAlO<sub>3</sub> to determine its role in the ferroelectric properties of the supercell.

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## Bio Symposia

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## This is a test title

**Author:** Corinne Allen<sup>None</sup>

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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 we were going to have a drop down menu for the type of submission.

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**Test****Author:** Francesca Toma<sup>None</sup>**Corresponding Author:** fmtoma@lbl.gov

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Blah blah blah

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test