

Molecular Foundry Conference and Abstract Call

Report of Contributions

Contribution ID: 0

Type: **Symposium - Making, Measuring and Manipulating****Two-Dimensional Matter**

Preparing AX2 compounds in a dry glove box.

PbCl₂, SnCl₂, BaCl₂ and BaI₂ all fall into a category of crystals known as AX₂ 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 AX₂ 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 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)