## ANSTO User Meeting 2021



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# Good vibrations: phonons in topological thermoelectrics

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Thermoelectric materials harness a temperature gradient to produce a voltage via the Seebeck effect, providing a way to harvest and recycle heat. Recently a new generation of thermoelectrics has been developed that offer unprecedented performance by leveraging topological physics. The key to their functionality is their robust high electronic conductivity in tandem with their low thermal conductivity. The latter can be engineered by controlling the lattice vibrations or "phonons". Here I will discuss recent neutron spectroscopy experiments at the Australian Centre for Neutron Scattering, ANSTO, which offer unique insights into the differences between "good" optical and "bad" acoustic phonon vibrations in thermoelectrics. I will show how these experiments are complemented by large-scale molecular dynamic simulations on the GADI supercomputer within the National Computing Infrastructure. Time permitting, I will also briefly demonstrate how we use the Centre for Accelerator Science and neutron reflectometry to enable surface-engineering in these novel crystals for microelectronic applications.

#### References:

N. Islam, D. L. Cortie et, Acta Materialia 215, 117026 (2021)W. Zhao, Cortie, Wang et al, Physical Review B 104 (8), 085153 (2021)D.L et al. Cortie Applied Physics Letters 116 (19), 192410 (2020)

## Level of Expertise

Experienced Researcher

## **Presenter Gender**

Man

#### Pronouns

He/Him

## Which facility did you use for your research

Australian Centre for Neutron Scattering

## Students Only - Are you interested in AINSE student funding

No

## Do you wish to take part in the Student Poster Slam

No

## **Condition of submission**

Yes

Primary author(s):Dr DAVID CORTIE, DavidPresenter(s):Dr DAVID CORTIE, DavidSession Classification:Physics, Surface & Condensed Matter

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