Misbehaving Materials: An ongoing computational investigation of rare-earth tritellurides (RTe_3, R = La-Lu) and charge density waves

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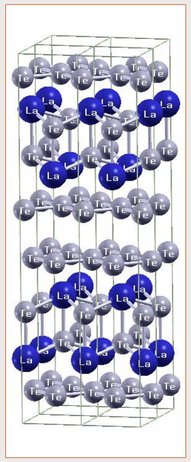
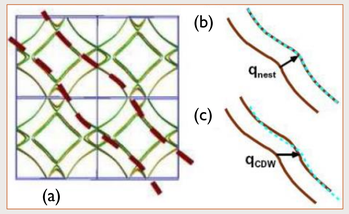
Background



Theoretical predictions for the formation of charge density waves (CDWs) in rare-earth tritellurides depend primarily on Fermi surfaces and their available nesting vectors. Experiments on these materials indicate that this theory is incomplete, and a suggested avenue for theoretical development considers the relationship between charge and lattice parameters[1].



Above: The unit cell for Lanthanum tritelluride. **Right**[2]: (a) Fermi surfaces, (b) nesting vector, and (c) CDW vector for $ErTe_3$

Methods

We conducted research using **Wien2K**, a program developed for density functional theory calculations, and we based our calculations on RTe_3, R = La.

Over the past semester we have completed the following tasks to launch our research:

- Optimization of lattice constants and atomic positions within the unit cell
- Implementation of calculations for density of states and electronic band structure for a range of a-lattice constants
- Qualitative investigation of changes in band structure and density of states over the selected range

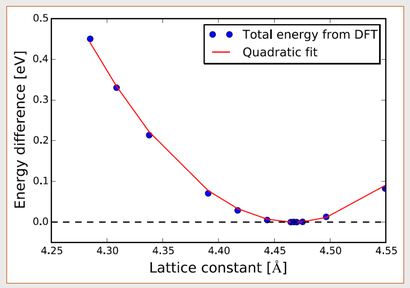


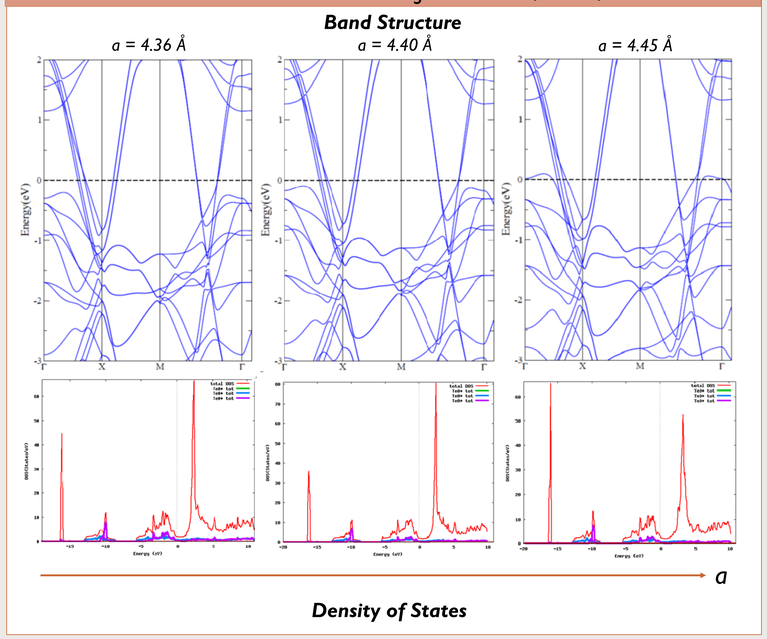
Figure: Energy minimization scheme for the selected lattice parameter and a quadratic fit.

Results

The optimized lattice parameters from which we proceeded were ***a* = *c* = 4.466 Å** and ***b* = 26.559 Å.** These values differ by <4% from experiment.

Our calculations generated band structures and density of states for the total Lanthanum tritelluride unit cell over a discrete range of lattice constants from a = 4.36 Å to a = 4.45 Å; a selection are shown below:

Electronic Calculations for $LaTe_3$; a = 4.36, 4.40, and 4.45 Å



Analysis

Lifshitz transition: Specific bands shift toward the Fermi level and even cross it by a = 4.45 Å, evidence of a topological change in the Fermi surface.

Top-layer distortion: Inspection of the bands links the Lifshitz transition to the tellurium atoms in the top layer, suggesting the CDW-associated electronic behavior depends on this tellurium layer and its coupling with lattice constant a. This may be related to steric hindrance[1].

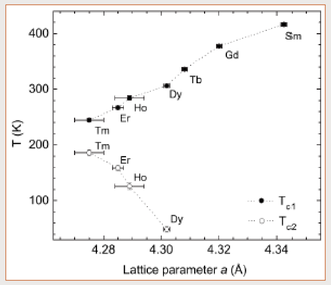
Future Research

Over the coming months we will continue this project by exploring the following areas:

- **Modulation of the *b*-lattice constant**—using the same approach outlined here with the long-axis in the unit cell
- **Charge density analysis**—paying close attention to charges associated with individual atoms; looking for charge transfer between layers
- **Expansion of the *a*-lattice constant investigation**—building from current findings for a-values currently uncalculated
- **Replacement of Lanthanum with Lutetium**—comparing the calculations for considerably different R in RTe_3 materials
- **Calculation of the Fermi surface**

Guided by experimentally-produced phase diagrams and more, we seek to understand the physical influences that affect the predictive power of Fermi surface nesting for RTe_3 CDWs.

Figure[2]: Phase diagram for RTe_3 materials, indicating key conditions for experimental emergence of CDWs.



Sources

[1] R. G. Moore, et al. , Physical Review B 93, 024304 (2016)
[2] N. Ru, et al., Physical Review B 77, 035114 (2008)

Acknowledgments

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