Calculating Phonon Energy when Changing the Central Atom of Barium Titanate, $BaTiO_3$.

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1. Summary

Here you should briefly summarize the work you would like to do. The three main ideas a proposal should communicate are: (1) Communicating novelty and/or importance of the study (why it should be done), (2) Explaining proposed work with specificity (what will be done), and (3) Methods and techniques to be employed (how it will be done). All three should appear briefly in the summary before appearing in more detail in the following sections.

This project will look at the allowed phonons within Barium Titanate, $BaTiO_3$, when changing out the central Titanium atom with other metals. The metals that are intended to be investigated will include Vanadium, Chromium and Manganese. Quantum Espresso will be employed to run simulations and calculations. The atoms proposed to replace the Titanium are the subsequent atoms to the right of Titanium on the Periodic Table. Changing the alloy composition will likely shift the allowed phonons with a trend related to some periodic trend.

2. Scientific Background

Here you provide the detailed explanation of why your research question is worthy of exploration. Communicating this idea will generally require a summary of (1) the current state of the field, (2) any gaps in understanding or currently unexplored terrain, and (3) how your work will fill that gap or improve the boundaries of our knowledge. This generally requires reference to the literature, and most of our citations of published work end up here.

For your project, it is too much to expect you to address all three. Rather, communicate for me (1) some background on the physical theory behind the property you are investigating, (2) at least one example of someone studying this property in a material and (3) a brief description of the material you would like to study.

Thermal energy and stress and strain forces within an atom cause waves that carry heat and sound through a system. Because these waves have definite energy and momentum, in quantum mechanical terms, they can be treated as a particle. This particle is called a phonon. Phonons can be thought of as a particle of heat and sound, the same way that photons are thought of as a particle of light. However, the waves associated with phonons will experience interference, while photons waves typically

don't. An example of phonons being studied is research done by Korrman et. al[1] on phonon broadening in high entropy alloys. The mass and force fluctuations in high entropy alloys induce significant phonon scattering and broadening. They investigated vibration energy through the changes in phonon scattering. The metals we would like to research are all similar to $BaTiO_3$, they all have cubic unit cells and five total atoms within each unit cell.

3. Proposed Research

In this section you detail your proposed research. Explain the specific research question you plan to investigate and the computational experiment you will perform to answer it. For example, you might consider how the displacement of Ti in $BaTiO_3$ affects the dielectric constant, and so you would describe the convergence testing you need to perform, specifically how you plan to shift the Ti location (along multiple axes or just one?), whether or not you are relaxing the other positions (or maybe you're going to do both), etc.

Close with your hypothesis, that is, what you expect to find, and a bit about why you expect this result.

We will investigate the change in allowed phonons in Barium Titanate as you replace the titanium with metals close in atomic number. We will replace the titanium with vanadium, chromium, and manganese.

As the atomic number of the replaced atom increases, the allowed energies of the phonons will increase.

4. Methods

Here you should describe each of the unique DFT calculations you need to perform. Each project will require performing at least one new type of calculation. You will need to look up the documentation or examples of performing this calculation and describe the parameters you will need to change to be able to perform the new calculation.

Quantum Espresso contains sufficient packets to complete the simulations required for this project as a standalone software. PHonon, phonons with Density-Functional Perturbation Theory is the initial packet intended to be used. Further packets may be employed to garner additional information as necessary. **Further research into what will be required is needed to fully flesh out this section**

References

[1].
phonon broadening in high entropy alloys.

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