# Article information:

First principles phonon calculations in materials science - ScienceDirect
[https://www.sciencedirect.com/science/article/pii/S1359646215003127?ref=cra\_js\_challenge=RR-1](https://www.sciencedirect.com/science/article/pii/S1359646215003127?ref=cra_js_challenge&fr=RR-1)

# Article summary:

1. This article discusses the importance of first principles phonon calculations in materials science and introduces an open source code, Phonopy, for such calculations.

2. Examples are given to demonstrate how the phonon calculations can be applied in materials science, such as calculating phonon band structure and density of states, thermal properties, atomic displacement parameters, and quasi-harmonic approximation.

3. The article also explains how crystal symmetry is utilized to improve numerical accuracy of force constants and reduce computational cost.

# Article rating:

Appears moderately imbalanced: The article provides some useful information, but is missing several important points or pieces of evidence that would be required to present the discussed topics in a balanced and reliable way. You are encouraged to seek a more balanced perspective on the presented issues by exploring the provided research topics and looking at different information sources.

# Article analysis:

The article “First Principles Phonon Calculations in Materials Science” provides a comprehensive overview of the use of first principles phonon calculations in materials science. The authors provide a detailed explanation of the theory behind these calculations and discuss their applications in various areas such as thermal properties, mechanical properties, phase transitions, and superconductivity. The authors also introduce an open source code called Phonopy which is used for these calculations.

The article is well written and provides a thorough overview of the topic at hand. However, there are some potential biases that should be noted when considering this article’s trustworthiness and reliability. For example, the authors focus primarily on the benefits of using first principles phonon calculations without discussing any potential drawbacks or risks associated with them. Additionally, they do not explore any counterarguments or alternative approaches to solving problems related to materials science that could be used instead of first principles phonon calculations. Furthermore, while they mention that their code has been widely used around the world, they do not provide any evidence or data to support this claim.

In conclusion, while this article provides a comprehensive overview of first principles phonon calculations in materials science and introduces an open source code for these calculations, it does not explore any potential drawbacks or risks associated with them nor does it present both sides equally by exploring counterarguments or alternative approaches to solving problems related to materials science that could be used instead of first principles phonon calculations.

# Topics for further research:

* Alternative approaches to materials science
* Risks associated with first principles phonon calculations
* Counterarguments to first principles phonon calculations
* Evidence for widespread use of Phonopy
* Advantages and disadvantages of first principles phonon calculations
* Comparison of first principles phonon calculations to other methods

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