Summary

In this experiment we will be looking at the variation of the dielectric constant of silicon as a function of volume. The dielectric constant is calculated using scf and eps calculations in DFT and plot results using Jupyter notebook. At the end of the project, we hope to get an insight about how silicon interacts with an electric field.

Background

Dielectric Constant is a measure of how much electrical energy a material can store. It can also be described as a measure of how polarizable a material is by an electric field. Mathematically, it is calculated as the ratio of permittivity and permittivity of free space.

Dielectric constant is affected by temperature, frequency of current, and free volume. Scientists like R Ramani are studying if free volume increases or decreases the dielectric constant of fluorine containing polyimide blend. The results show an increase in the dielectric constant of the material owing to the availability of more free volume (Ramani, 2015). This is an interesting experiment that had many variables due to the nature of the material studied.

Olivia and I hope to do an experiment on a similar idea, examining the effect of free volume on dielectric constant. However, we will use silicon for simplicity. Silicon is a crystalline metalloid. It is found below carbon in the periodic table and has four valence electrons. Therefore it is capable of forming a stable tetrahedral configuration (LibreTexts, n.d.). In this configuration, each silicon atom is bonded with four atoms. That leaves no electrons in the valence band, making for a good insulator.

Proposed Research

Ethiopia and I will see how increasing or decreasing the free volume of a silicon molecule changes its dielectric constant. If time allows we will change other or more specific volumetric parameters and see how they affect the dielectric constant. We will perform DFT (density functional theory) calculations for the dielectric constant with quantum espresso using atomic spacing as our variable. We believe by increasing the free volume of the silicon molecule we will see an increase in the dielectric constant because “opening up” the molecule may allow more room for electricity to flow.

Methods

We will do multiple DFT calculations using quantum espresso. Firstly a scf calculation to set things up, mainly changing the number of bands and turning off crystal symmetry. Then we will do an epsilon.x calculation to actually get the dielectric constant values. We will do this for at least five different atomic spacings. We will then plot our

dielectric constant of silicon as a function of free volume by uploading our data to jupyter notebooks.

References

Ramani, 2015 Direct correlation between free volume and dielectric constant in a fluorine-containing polyimide blend https://iopscience.iop.org/article/10.1088/1742-6596/618/1/012025/pdf#:~:text=The%20dielectric%20constant%20of%20fluorinated,polarizable%20groups%20per%20unit%20volume.

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