

student summaries and exam question suggestions

geometry optimization (part 1)

*These pages contain student summaries for the module **geometry optimization (part 1)**, as well as student suggestions for exam questions on this module. You can use these pages as a study help for this module. The summaries can help you to see the highlights of this module from different points of view. The questions can challenge you to think about the content. If you take the exam, then some of the questions suggested this year will be included in the exam. The contributions suggested this year are **are printed in color**. The ones in black were contributed in previous years.*

1. student summaries

- even though we will just be using the vc-relax for doing the geometry optimizations later in the course, it is important to understand what the manual procedure would be to do the same thing, what the degrees of freedom are in the unit cell and how they can vary according to the symmetry of the cell.
- For the initial guess of the equilibrium properties of a crystal we can use the Birch-Murnaghan equation. But, if we want accurate values we should use the full optimization (ev.x)
- How to determine the optimal volume, the pressure and bulk modulus
- How several parameters (like the pressure) can be calculated in different ways
- What is a geometry optimisation, what is an E(V) curve, how is the bulk modulus calculated from this curve, what about pressure.
- How to determine shape and volume using quantum espresso
- In the first part of this lecture we discussed how to perform a volume optimization using dft. In this discussion we talked about the Murnaghan equation and how this can be useful for the optimization. Next we talked about the relevance of the bulk modulus in geometry optimization and discussed the difference between the Birch-Murnaghan and the Murnaghan equations of state. And finally we looked at how we can change and study the effects of changing the cell shape using dft.
- What the bulk modulus is. How to optimize a crystal. What parameters can be influenced to optimize a crystal.
- Calculating datapoints and doing fits in quantum espresso
- The treating of solids via an equation of state and reading out such equations' parameters in the context of DFT simulations should be remembered from this week. First steps towards full geometry optimisation were covered.
- The properties of solids depend a lot on the geometrical disposition of atoms, and it is very important to study which configurations are energetically favoured
- - (Birch-)Murnaghan equation - How to use the ev.x tool
- DFT can predict material properties.
- The cell volume and cell shape can be optimized in terms of an energy minimization. The pressure or energy as a function of the cell volume can be described as an equation of state, namely the Murnaghan equation. The more precise form is the Birch-Murnaghan equation.
- Geometry optimization uses small deviations in cell parameters to minimize the energy. The first way is to find the cell volume that gives the minimal energy. Second is cell shape. How one finds bulk modulus through the volume optimization, and the various fits used for the E(V) graphs.
- This week was more hands-on than the previous week. The key takeaways are the volume and cell shape optimization of a crystal.

2. exam question suggestions

- Given a unitcell and a cif file, explain what the degrees of freedom are and explain in a simple procedure how a the geometric optimization procedure would look like (what to vary and in which order) if you had to do it manually.
- How is the bulk modulus B expressed at any other volume (or pressure)?
- What info can you get from an $E(V)$ curve?
- What types of fits could be used for what kinds of data/curves?
- How is the $E(V)$ curve related to pressure?
- PbSO4 crystal
- Give the definition of the Bulk modulus.
- How do we determine which crystal structure is the most optimized? What parameters can we influence to further optimize it?
- Given a crystal, optimize its volume with quantum espresso
- What is, in general terms, an equation of state? Indicate how you would obtained its parameters of a solid crystal, assuming you are given simulation data of your choice.
- Given $E(V)$, estimate the preferred volume.
- What material properties van DFT predict?
- Qualitatively describe what the Birch–Murnaghan equation stands for.
- How can you determine the pressure needed to reduce the volume to a certain volume?
- Describe the role volume optimization and what its uses are. Can we obtain information about the solid from the result?
- What is the Birch-Murnaghan fit and for what is it useful?