Introduction to the Theory of Lattice Vibrations and their Ab Initio Calculation

Lecture 8: Hands-on tutorial on the SSCHA method

Ion Errea

Dept. Applied Physics, University of the Basque Country (UPV/EHU), San Sebastian, Spain

Centro de Fśica de Materiales (CSIC-UPV/EHU), San Sebastian, Spain

Donostia International Physics Center, San Sebastian, Spain

University of Science and Technology Beijing

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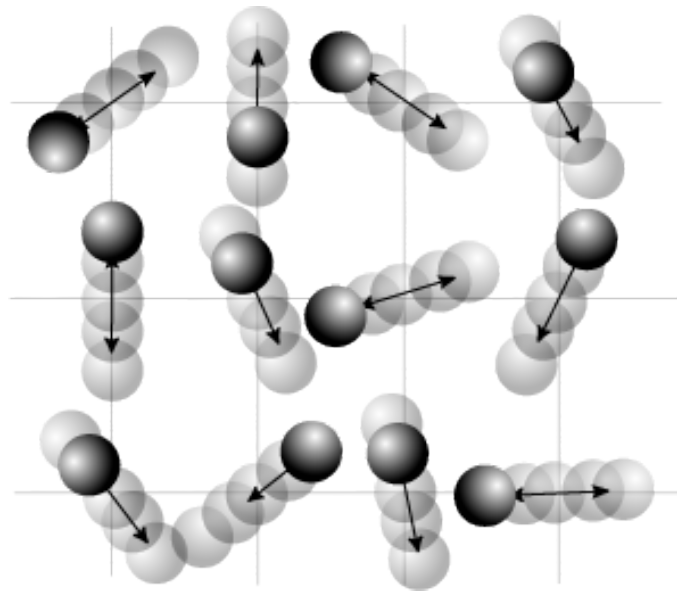

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Universidad del País Vasco

Euskal Herriko Unibertsitatea

CFM Materials Physics Center

Centro de Física de Materiales

Materialen Fisika Zentroa

Donostia International Physics Center

REMARKS BEFORE STARTING:

This tutorial is meant to lear some basic usage of the SSCHA code. The tutorial is based on three folders

- Lecture8_SSCHA_Tutorial/PbTe_simple_example_ab_initio/
- Lecture8_SSCHA_Tutorial/PbTe_cell_relax_ab_initio/
- Lecture8_SSCHA_Tutorial/SnTe_Force_Field/

In this folders you will get the input files. A calculation that I have ran can be found in Lecture8_SSCHA_Tutorial_Output, which can be used as a reference of how the calculations are expected to behave.

Sotwfare needed to run the hands-on tutorial

1. **SSCHA**:
   website: `http://sscha.eu/`
   installation: `http://sscha.eu/download/`
   install CellConstructor, python-sscha, F3ToyModel
   The easiest installation mode is to use pip. This is valid for CellConstructor and python-sscha. The F3ToyModel needs to be downloaded and installed with the command python setup.py install
2. **Quantum Espresso**:
   It will be used to ruun the force calculations on supercells website:
   `https://www.quantum-espresso.org/`
   installation and download: `https://www.quantum-espresso.org/login/`
3. **Python**:
   It will be necessary as the python-sscha is written in Python
4. **ASE**:
   It will be used by the SSCHA
   website: `https://wiki.fysik.dtu.dk/ase/`
   installation: `https://wiki.fysik.dtu.dk/ase/install.html`

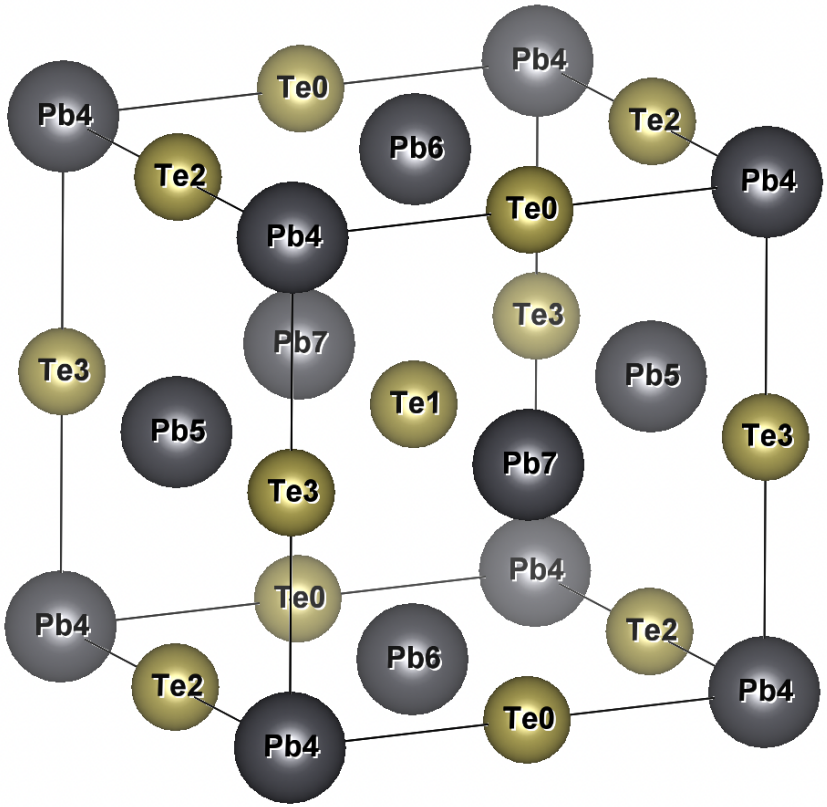
Outline

PbTe ab initio complete example

- A polar insulator, with a rock-salt structure ($Fm\bar{3}m$ (225) space group)
- Wyckoff positions:
  - Wyckoff positions

    Pb 4a $(0, 0, 0)$

    Te 4b $(1/2, 1/2, 1/2)$
- A structure close to a lattice instability, ferroelectric transition



PbTe ab initio complete example

We are going to perform a SSCHA minimization calculating the energies, forces, and stress tensors with DFT using Quantum Espresso

- Perform a SSCHA minimization on a $2\times2\times2$ supercell. We will create populations (ensembles) as much as needed to converge the gradient. An extra population with more configurations will be performed in the end to check the stochastic convergence.
- The free energy Hessian will be calculated as post-processing
- The spectral function will be calculated at Γ and in a path of the Brillouin zone
- Python scripts will be used to run the SSCHA code

PbTe ab initio cell relaxation

- In the second example we will see how the SSCHA minimization can be ran to minimize the lattice parameters of a given structure including quantum anharmonic effects in the stress tensor
- The minimization will not be run with a python script, but as an stand-alone code with an input file

SnTe force field calculation

In the third example we will see how the structure changes in a system due to quantum anharmonic effects. The model system will be $R3m$ SnTe, which due to quantum and thermal anharmonicity symmetrizes into a $Fm\bar{3}m$ crystal

- The calculation is performed with a python script setting up an ASE calculator with the force field
- The minimization is performed without storing the ensembles
- The minizaton in one script is able to run more than one minimization in the automatic mode