

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

Lecture 0: Details of the Course

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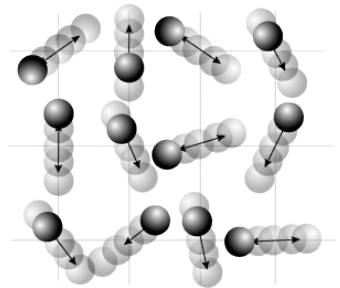
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- 1 Electrons and Ions in Solids
- 2 Classical Theory of Lattice Vibrations
- 3 Quantum Theory of Lattice Vibrations
- 4 Calculation of Harmonic Phonons with DFT or Other Methods
- 5 Hands-on Tutorial on the Calculation of Harmonic Phonons with DFT
- 6 Measuring Phonons and the Problems of the Harmonic Approximation
- 7 Anharmonicity Beyond Perturbation Theory: the SSCHA method
- 8 Hands-on Tutorial on the SSCHA
- 9 Quantum and Anharmonic Effects on DFT or Other Methods Superhydrides
- 10 CDW and Ferroelectric Transitions

- 1 Lectures and hands-on material will be available at:
<https://ehubox.ehu.eus/s/LXtmHSbgrbQxa24>
- 2 You can contact me at:
ion.errea@ehu.eus

Software needed to run the hands-on tutorial

- 1 **Quantum Espresso:**
website: <https://www.quantum-espresso.org/>
installation and download: <https://www.quantum-espresso.org/login/>
- 2 **Python:** will be used for plotting
matplotlib
numpy
- 3 **PHONOPY:**
website: <http://phonopy.github.io/phonopy/>
installation: <http://phonopy.github.io/phonopy/install.html>
- 4 **SSCHA:**
website: <http://sscha.eu/>
installation: <http://sscha.eu/download/>
install CellConstructor, python-sscha, F3ToyModel