Density Functional Theory

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Quantum Mechanics

Schrödinger equation $$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \hat{H}\Psi(\vec{r},t)$$

Hamiltonian $$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r},t)$$

Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p_i}^2}{2m_i} + V(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, t)$$

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N} \nabla_i^2 - \frac{1}{2}\sum_{k=1}^{M} \nabla_k^2 - \sum_{i=1}^{N}\sum_{k=1}^{M} \frac{Z_k}{r_{ik}}$$

$$+ \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}} + \sum_{k=1}^{M}\sum_{l>k}^{M} \frac{Z_k Z_l}{R_{kl}}$$

Born-Oppenheimer approximation

- The nuclei are much heavier than the electrons and move more slowly than the electrons

- In the Born-Oppenheimer approximation, we freeze the nuclear position and calculate the electronic wave function and energy

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N}\sum_{k=1}^{M}\frac{Z_k}{r_{ik}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}}$$

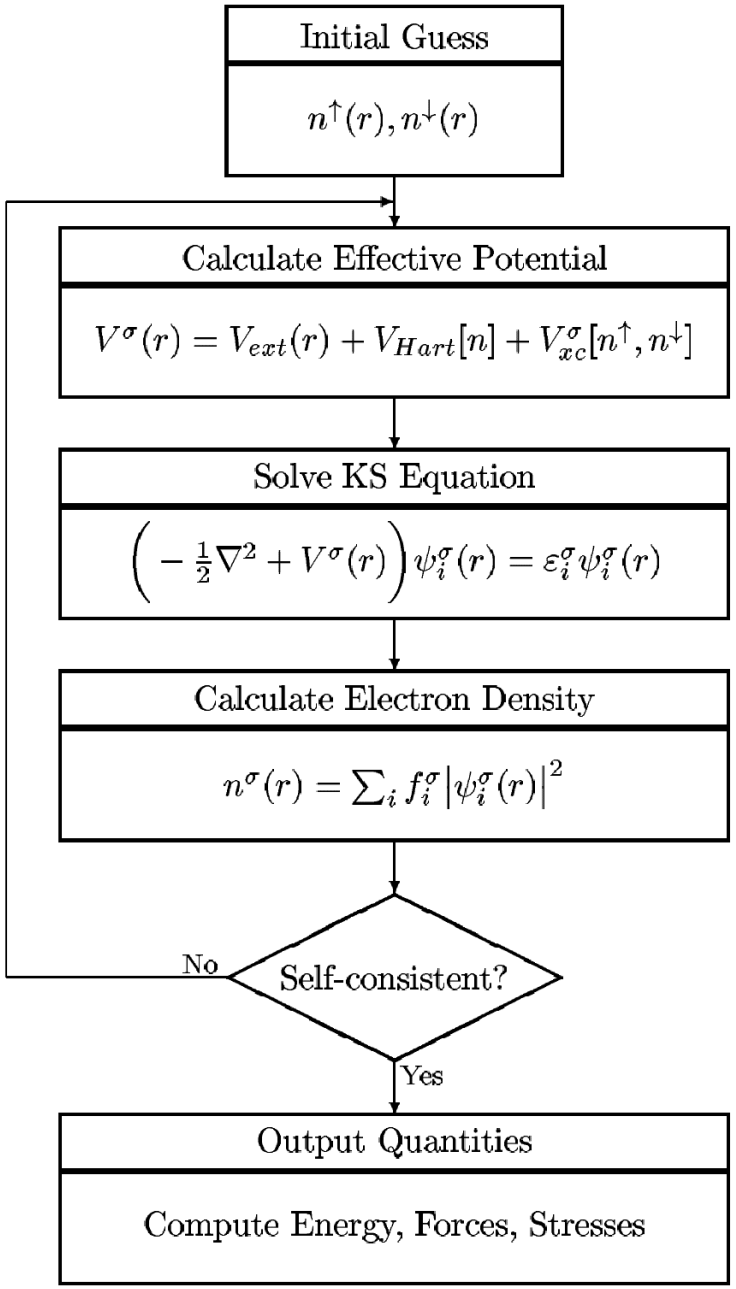
The Kohn-Sham Ansatz

$$n(\vec{r}) = N \int d\vec{r}_2 ... \int d\vec{r}_N \psi^*(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)\psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$$

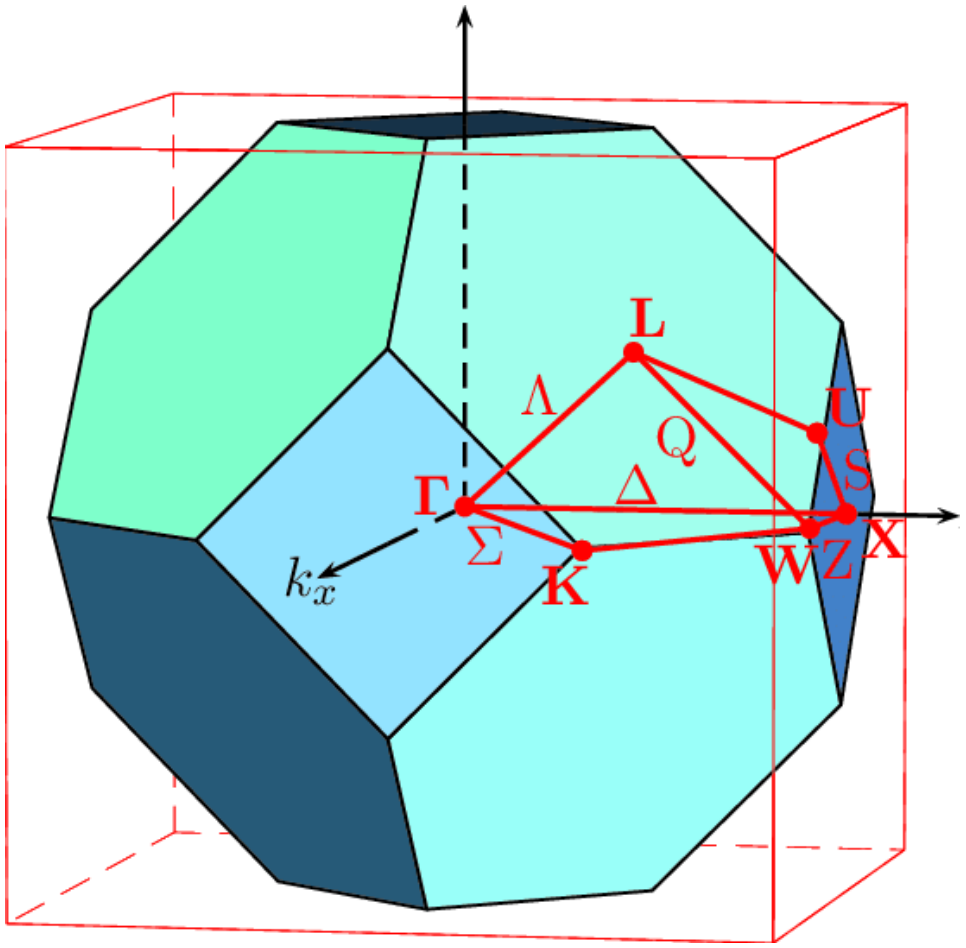
$$E[n] = T[n] + E_{Hartree}[n] + \int dr V_{ext}(r) n(r) + E_{xc}[n]$$

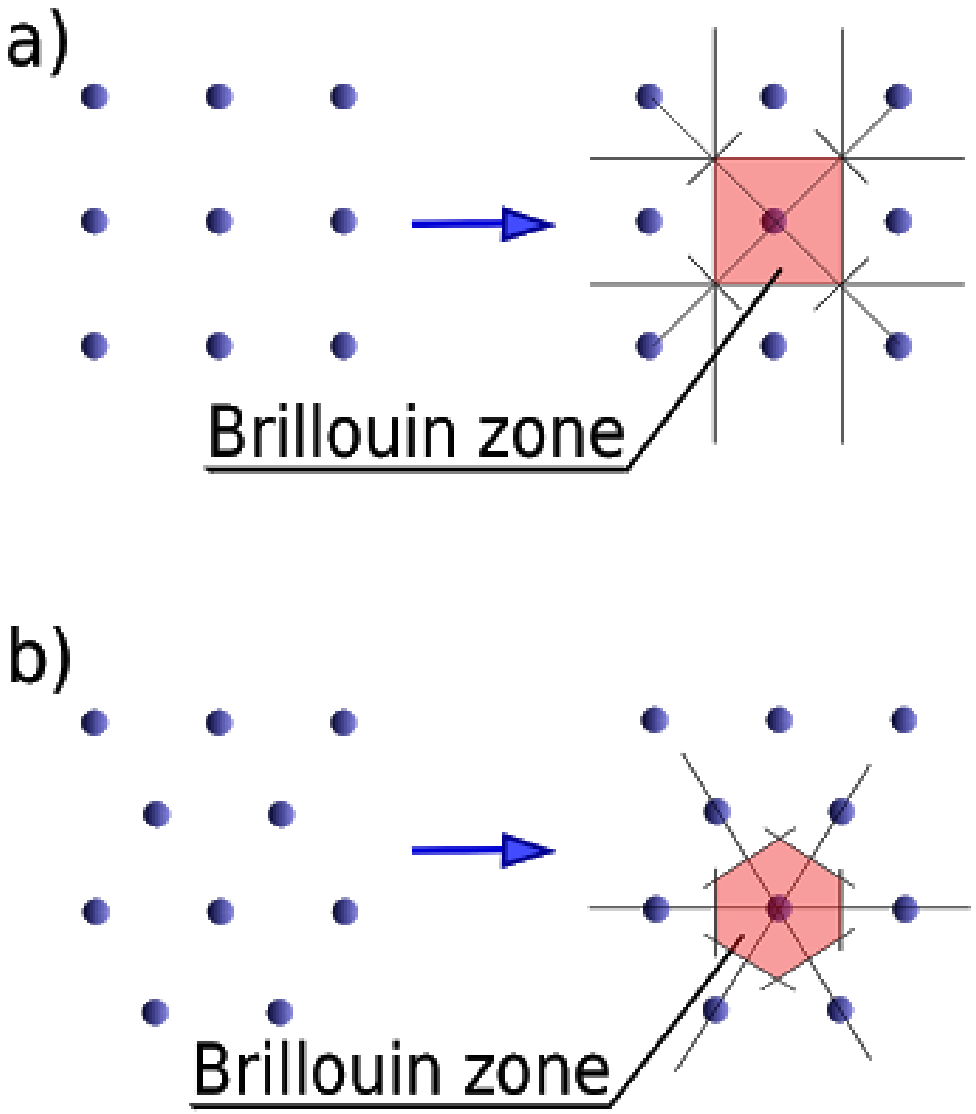
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r) + V_{Hartree}(r) + V_{xc}(r) \right) \psi_i(r) = \varepsilon_i \psi_i(r)$$

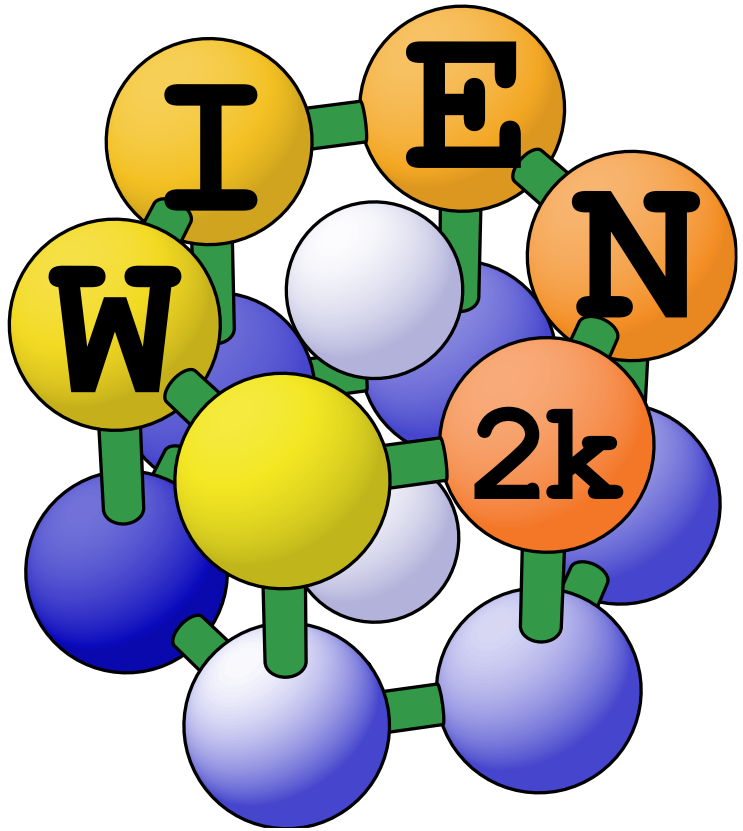
Kohn-Sham equations



Brillouin zone







WIEN2k Tutorials

tiny.cc/w2k

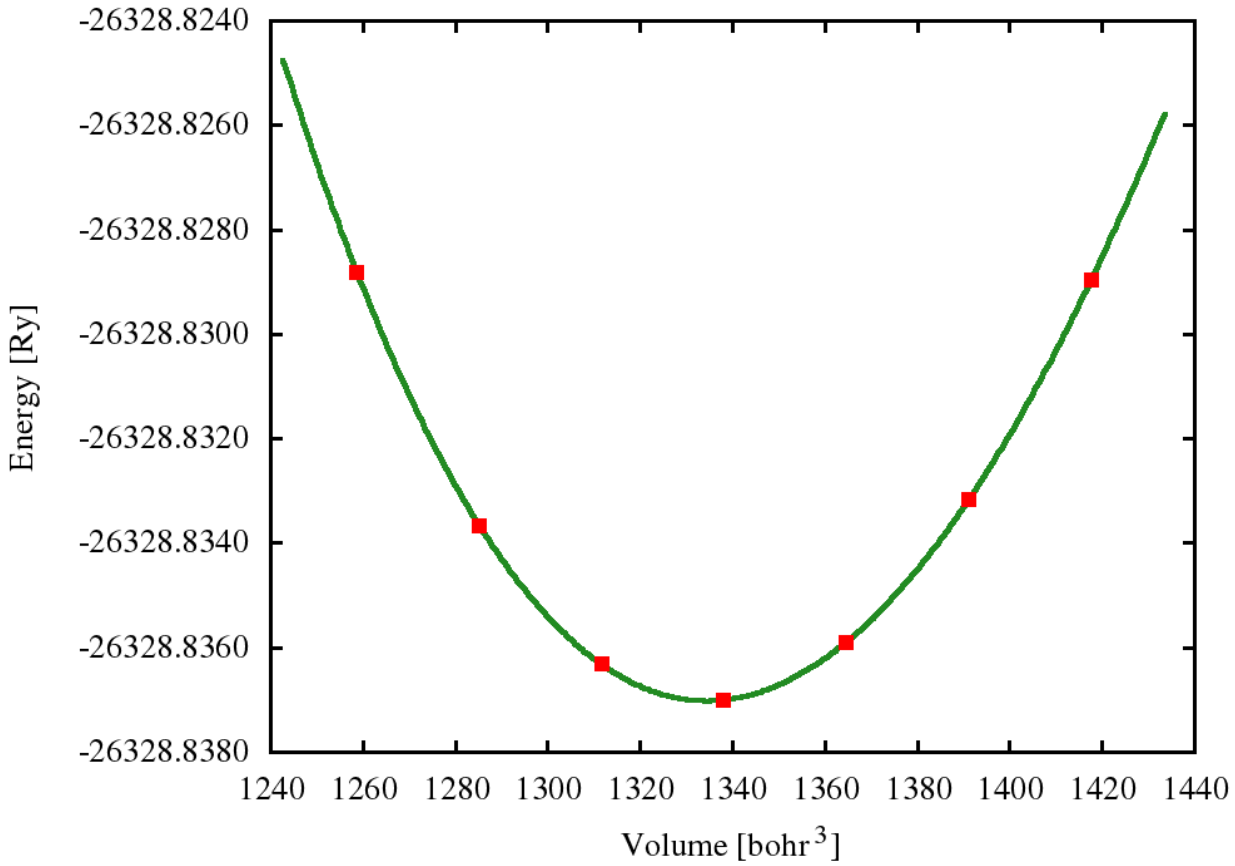
Calculation steps

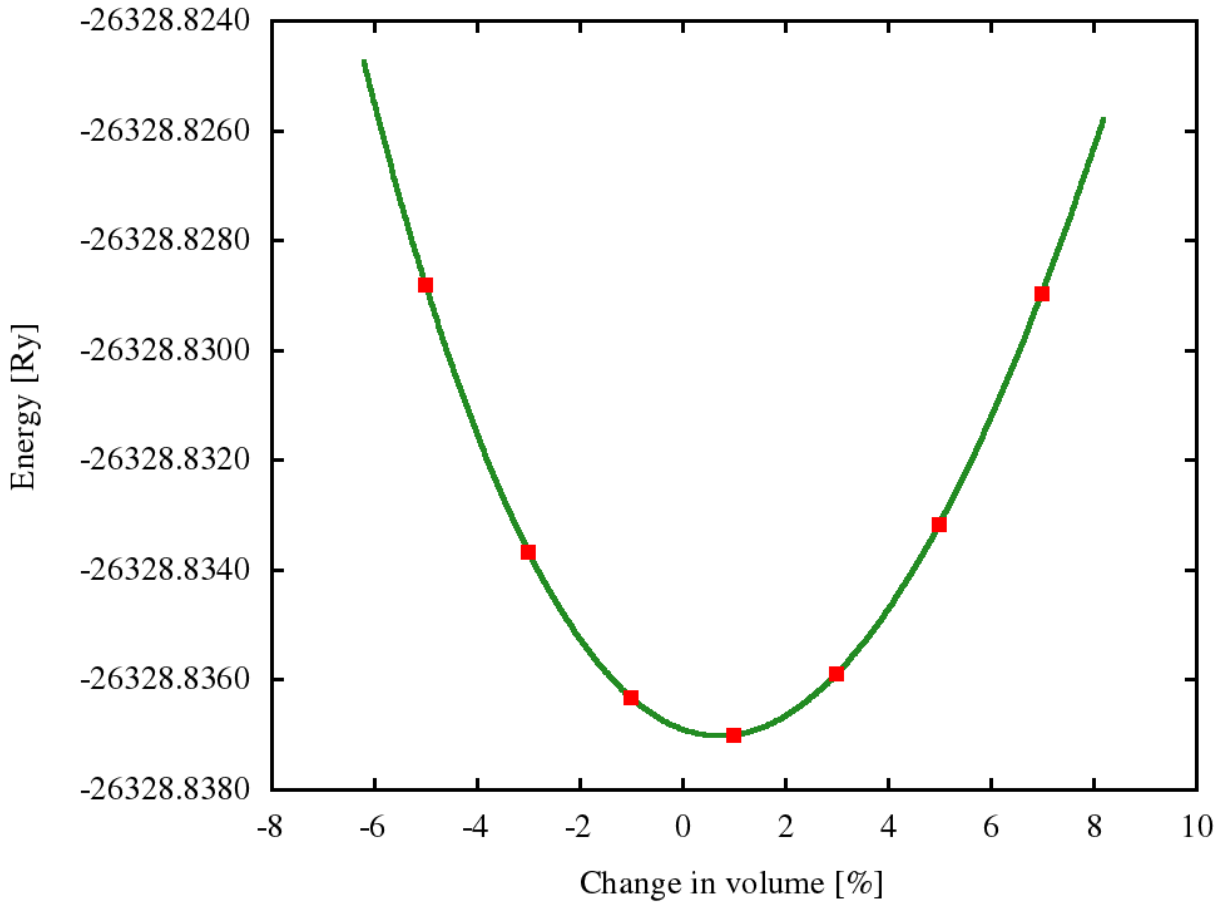
- Generate structure
- Initialize calculation (prepare input files)
- Make a test run [run(sp)_lapw –i 1]
- Volume optimization (use my script to save the results)
- Select the low energy structure (may need to change the lattice parameter)

Calculation steps

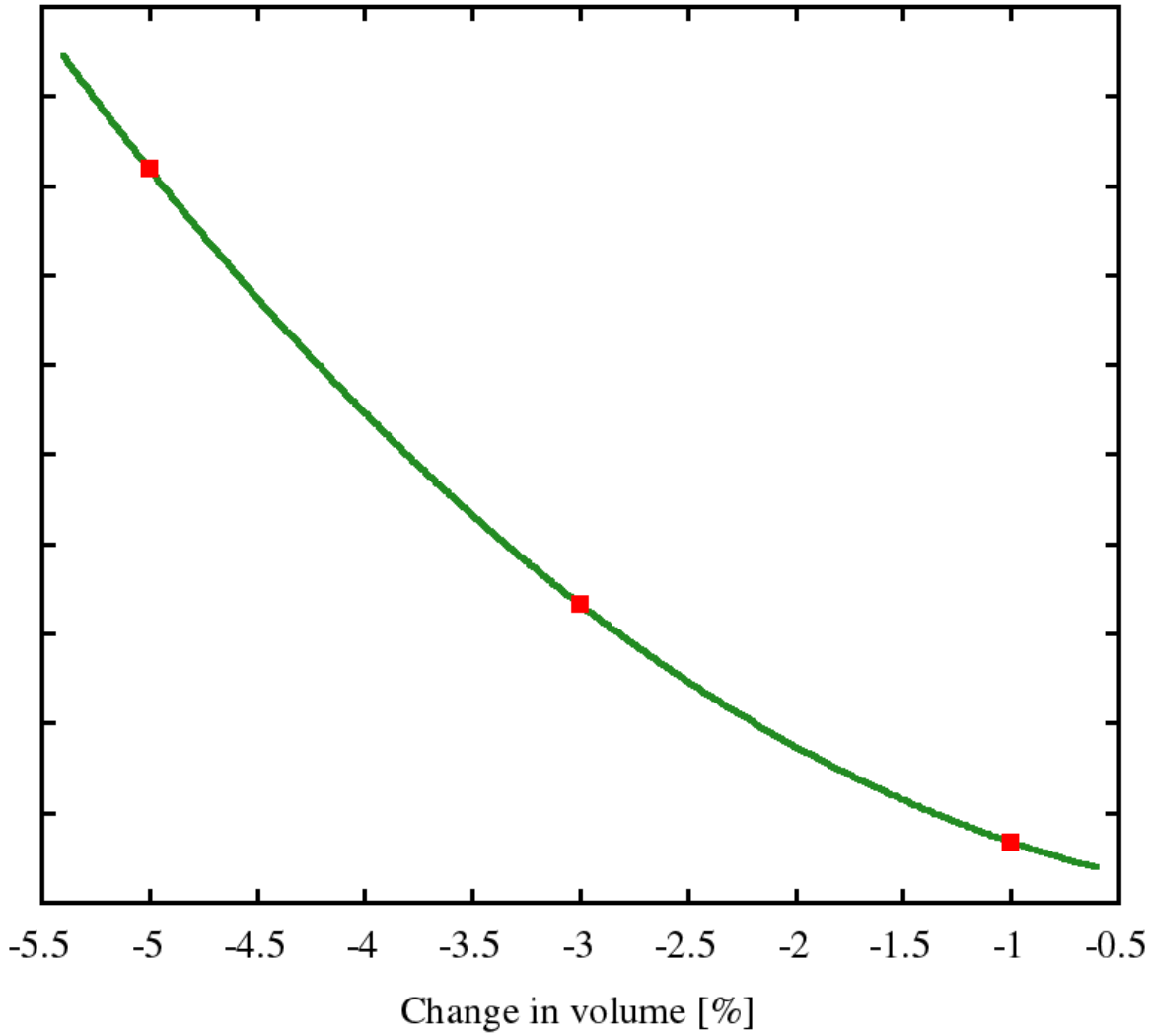
- Initialize calculation (prepare input files)
- Perform SCF calculation
- Save the results (use my script)
- Calculate DOS and PDOS
- Calculate optical properties
- Calculate band structure

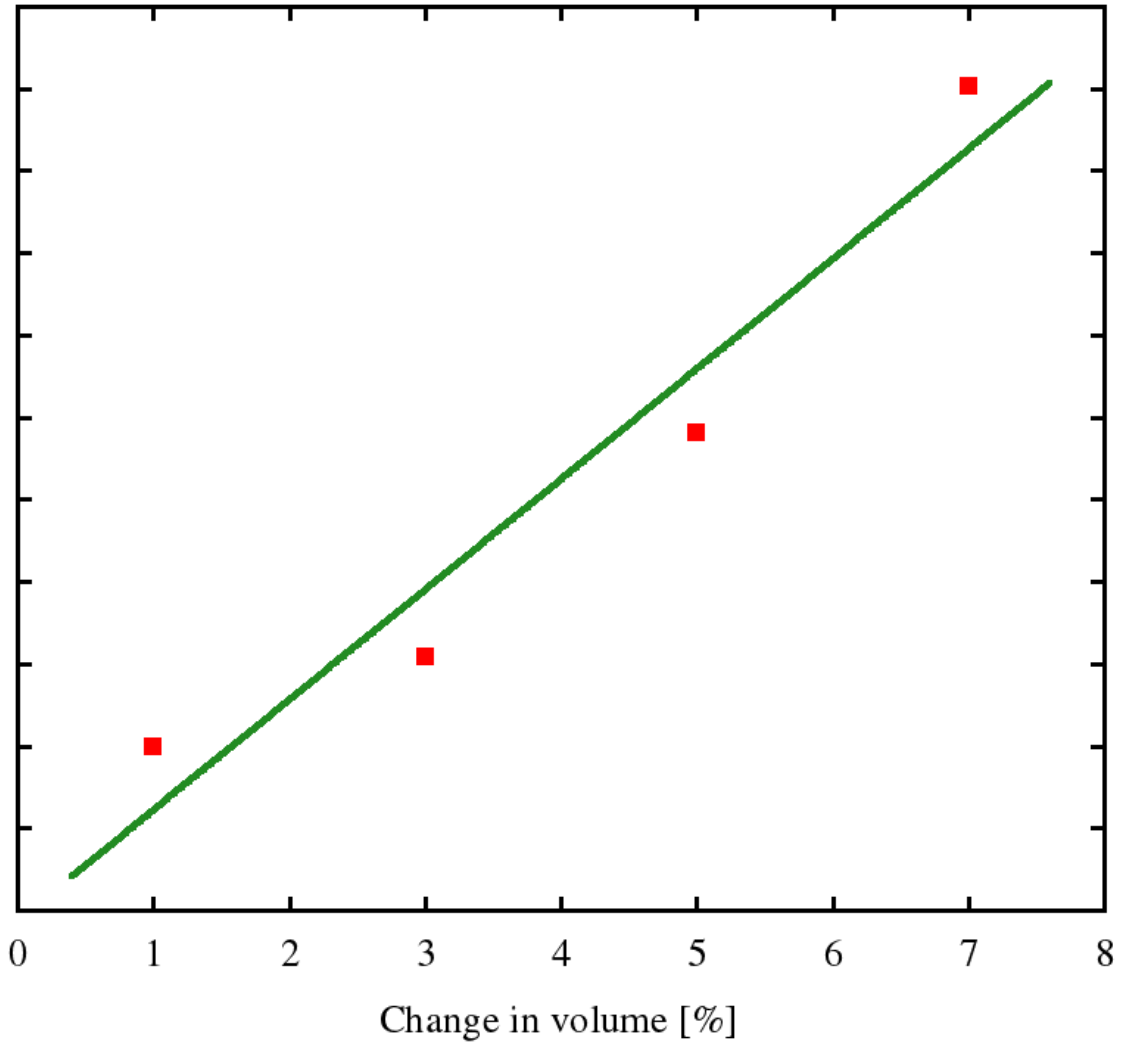
Volume optimization



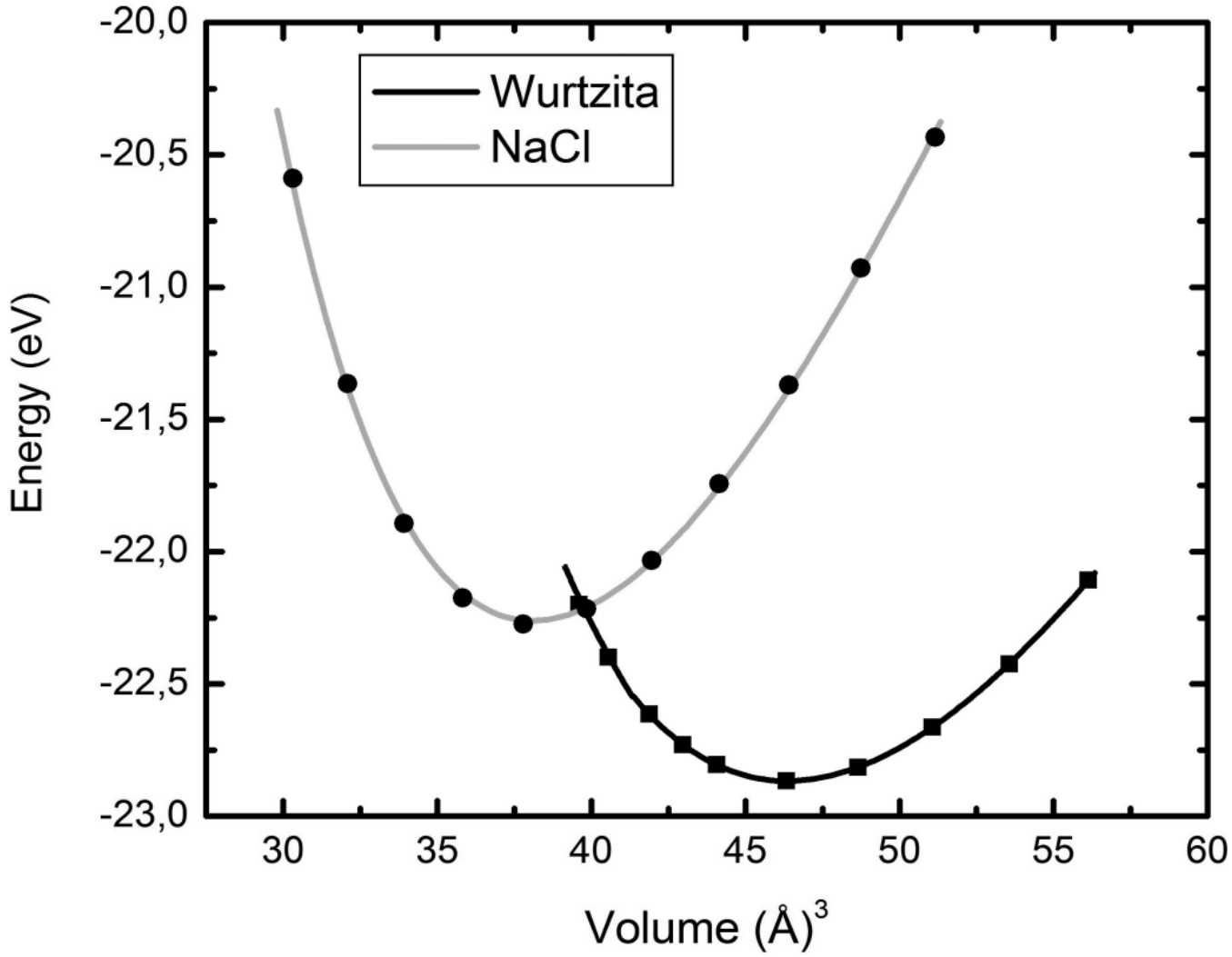


Volume optimization

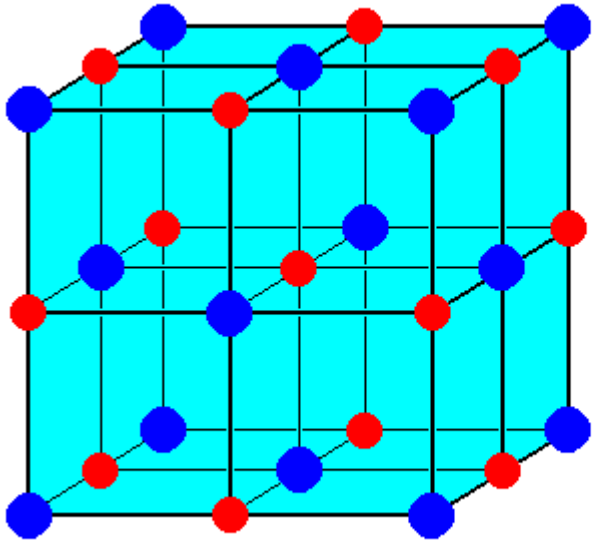




Volume optimization



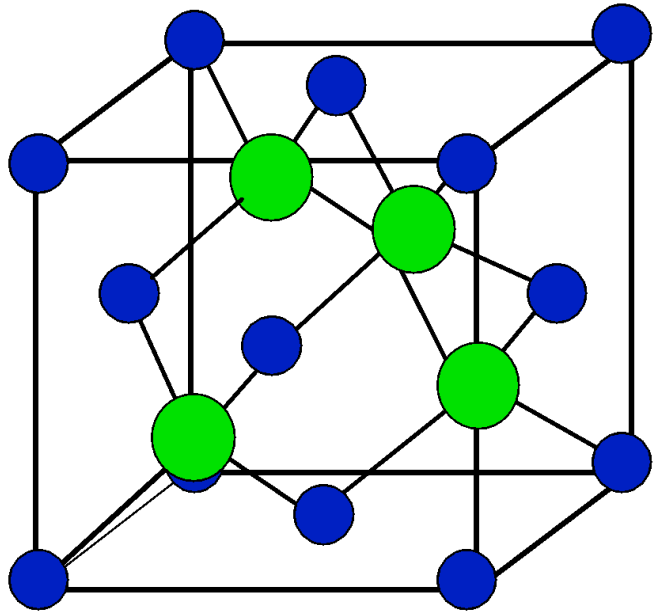
Structure



Cl^-

Na^+

NaCl



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Writing project report

- Introduction
- Theory
  - Basic Quantum Mechanics
  - Density Functional Theory (DFT)
- Results and Discussion
- Conclusion

Abstract

Introduction

- Introduce your system
- Why the system is interesting/important
- Briefly write about the methodology (DFT)
- Write about WIEN2k
- Structure of your report

Theory: Basic Quantum Mechanics

- Schrödinger Equation
  - Single particle
  - Many-body system
- Wave function
- Born-Oppenheimer approximation
- Hartree-Fock approach
  - Limitations of HF approach

Theory: Density Functional Theory (DFT)

- Electron density
- Thomas-Fermi model
- Hohenberg-Kohn Theorem
- Kohn-Sham Equation
  - Flow chart
- Exchange-correlation functional

Results and Discussion

You may describe in several chapters (with appropriate name) depending on your calculations and results

- Crystal structure
- Calculation parameters
- Optimization
- SCF calculation
- Electronic, magnetic, optical, structural, mechanical properties

Conclusion

Last but not least

Bibliography

What you can NOT do!

- Do NOT copy without proper reference
- Do NOT copy world-by-world even with reference
- Do not repeat word for word the abstract, introduction or discussion
- Be factual and orderly, but try not to be too dry

https://www.ldeo.columbia.edu/~martins/sen_sem/thesis_org.html


Thank You