Computing Vibrationally Averaged X-Ray Spectra

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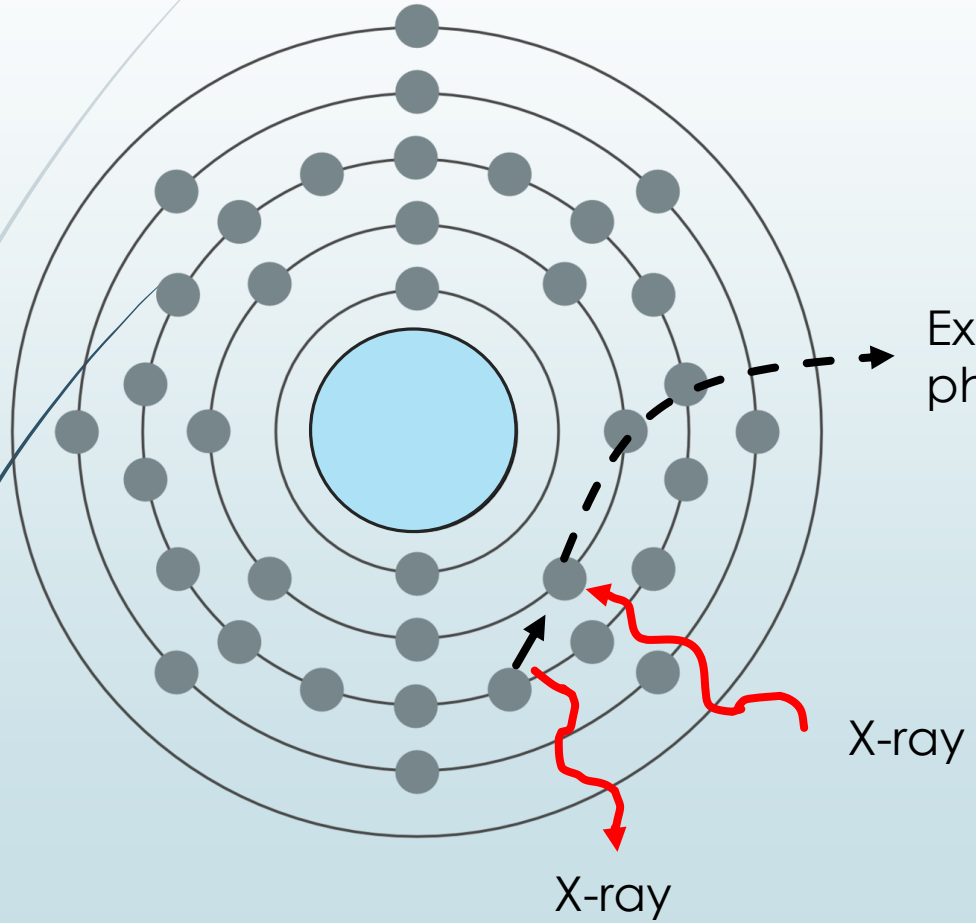
Agenda

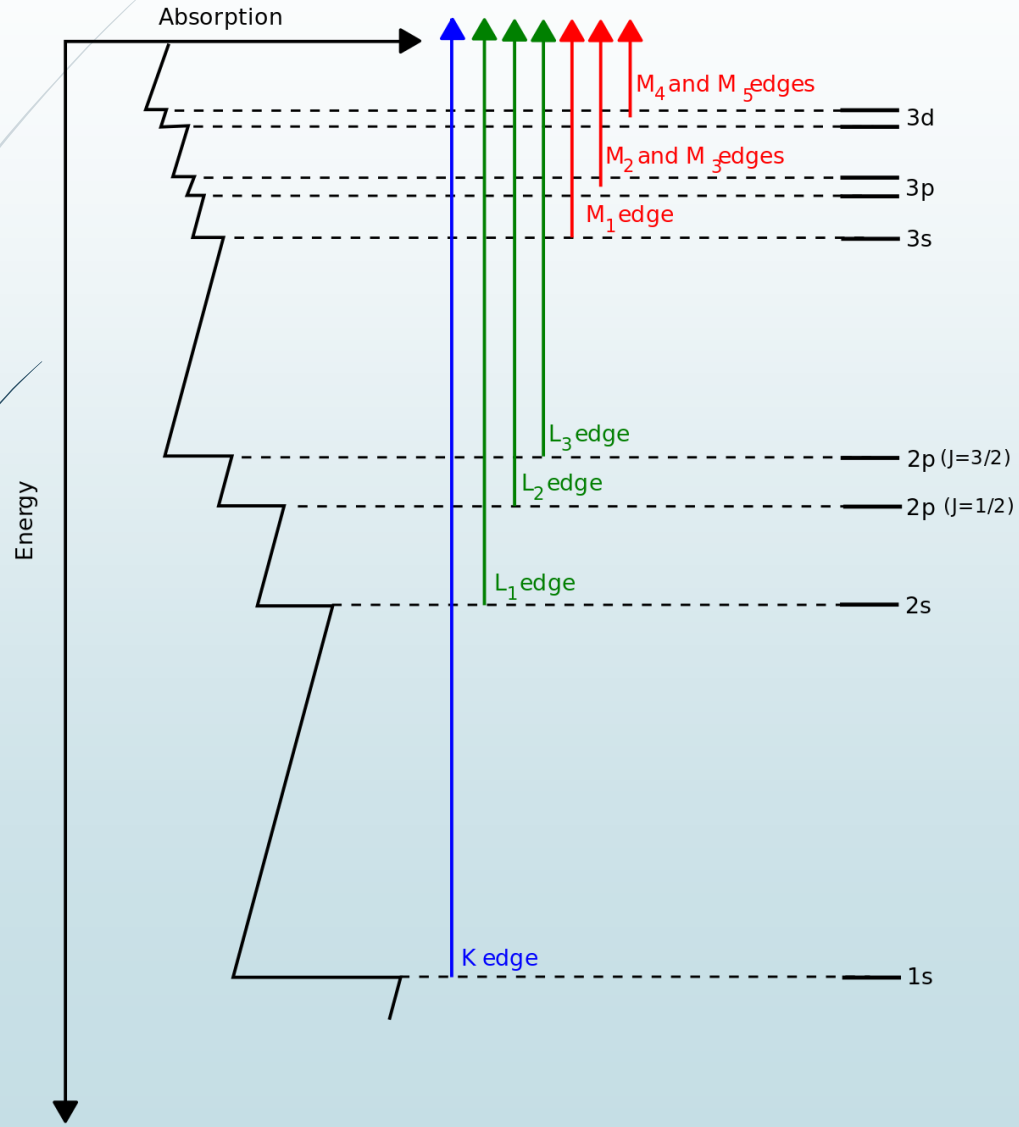
- Background
  - X-ray Spectroscopy
  - FEFF-9
- Main Project
  - Proper Thermal Distortions
  - Inverse Transform Sampling
  - Producing the Spectra
- Conclusion

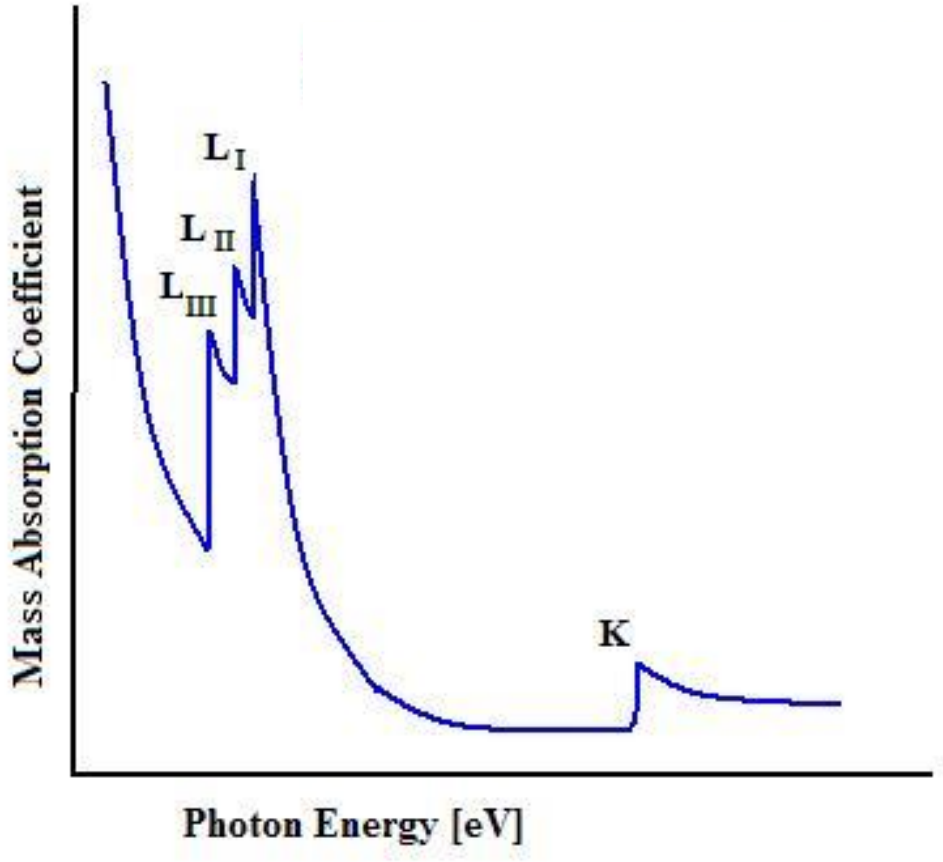
X-ray Absorption Spectroscopy

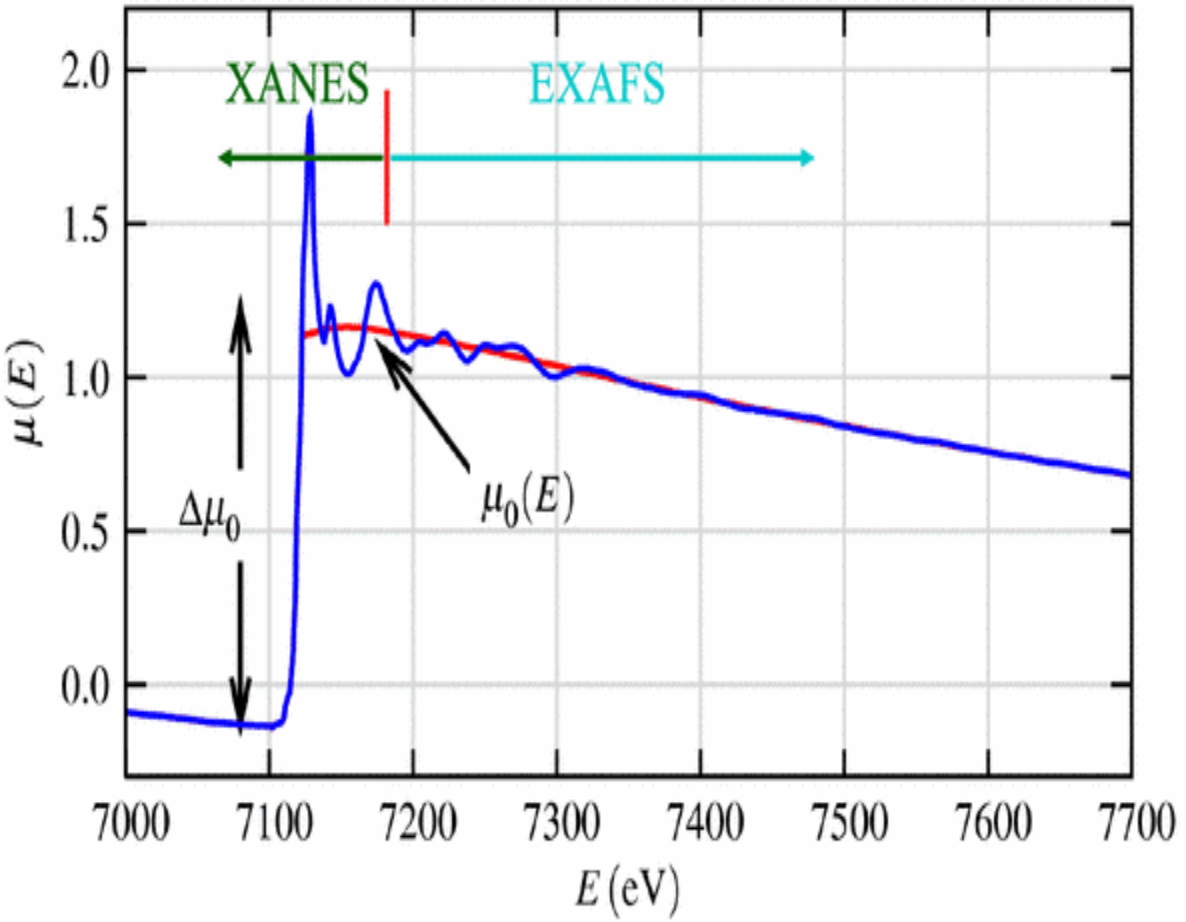


1) Incoming X-ray
2) Deep-core electron is promoted above fermi energy
3) This leaves a core-hole
4) Later, a higher electron takes its place
5) Emitted Photon

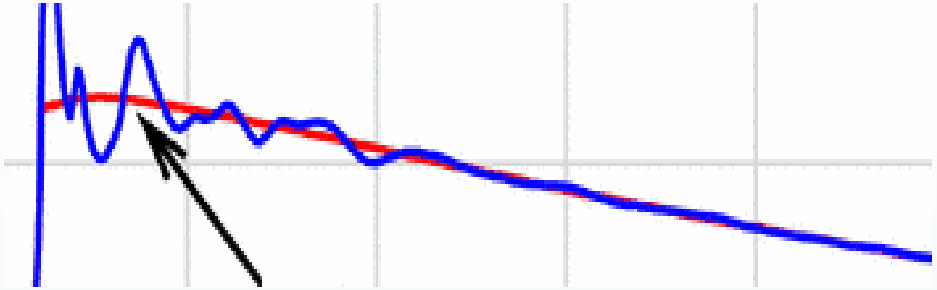
X-ray Absorption cont.




Mass Absorption Coefficient
L I
L II
L III
K
Photon Energy [eV]


XANES
EXAFS
2.0
1.5
1.0
0.5
0.0
μ(E)
Δμ0
μ0(E)
7000
7100
7200
7300
7400
7500
7600
7700
E (eV)

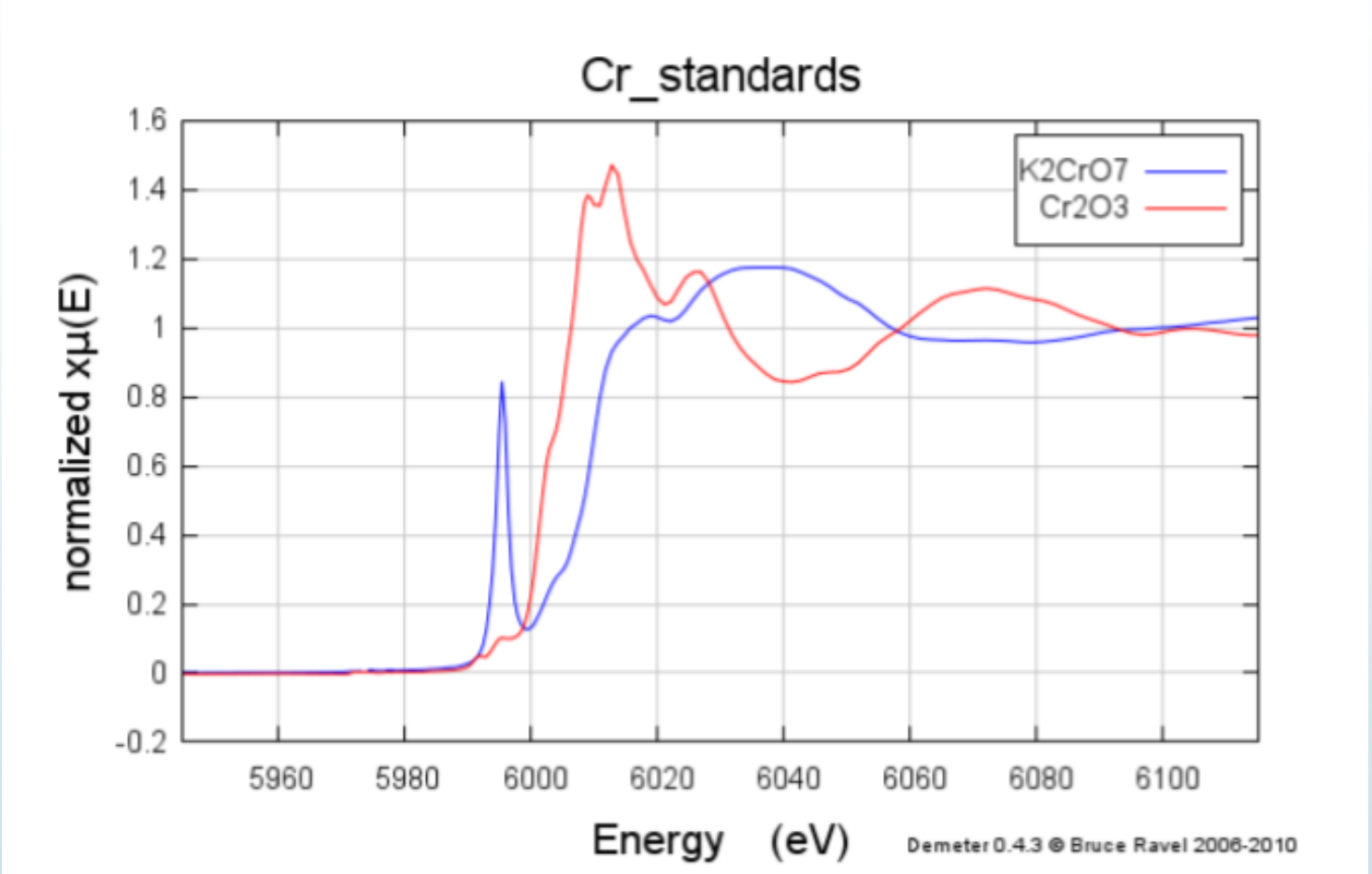
EXAFS



- Extended X-ray Absorption Fine Structure
  - What occurs once core hole is filled.
  - No available state, No absorption
  - Ejected photoelectron scatters with neighbors

XANES

- X-ray Absorption Near Edge Structure
- Fingerprint of a particular chemical



Debye Waller Factors

- Describes attenuation of x-ray scattering
- Damping factors caused by vibrations of atoms
- Thus basic expression for DWF relies on displacement of atom centers

FEFF


Fernando Vila
Keith Gilmore
Josh Kas
Igor Clevac
Eric Lentz
Kevin Jorissen
John Rehr, P.I.
Shauna Story
Andrew Lee

My Project Goals

- Currently, DWF calculated then used as a parameter
- For XANES, there are cases where it is greatly approximated and can lead to big errors
- Proposal: Incorporate DWF for XANES using probability functions
  - Computationally faster
  - Greater Accuracy

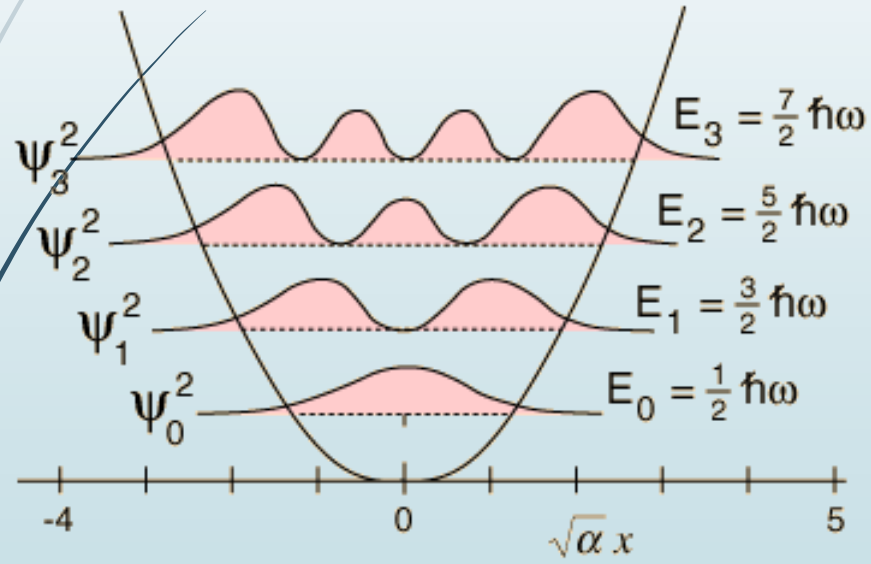
Make The Plan

1. Calculate PDF with H.O. approximation
2. Include proper thermal distortions according to BE distribution
3. Inverse Sample points to generate probability amplitudes.
4. Use probability amplitudes to shift atoms' positions
5. Generate XANES spectrum for every point and average them

Final: "Compute Vibrationally Averaged X-ray Spectra"

Execute the Plan

1. Calculate PDF with H.O. approximation

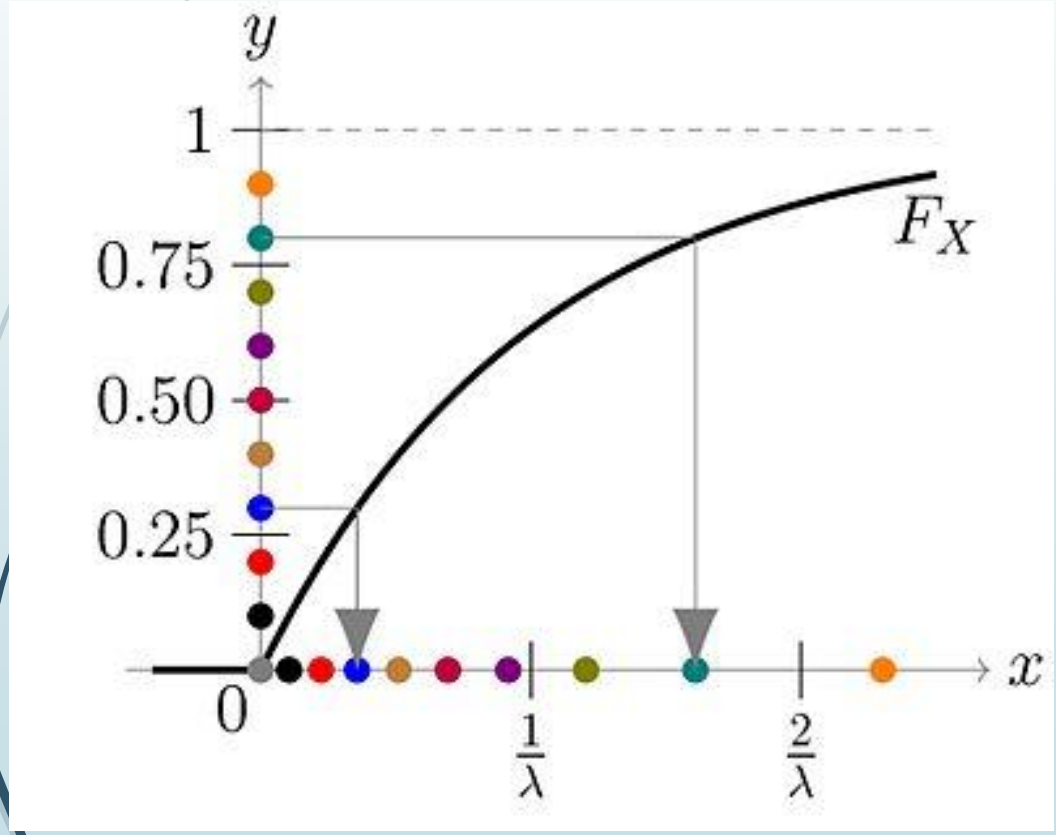


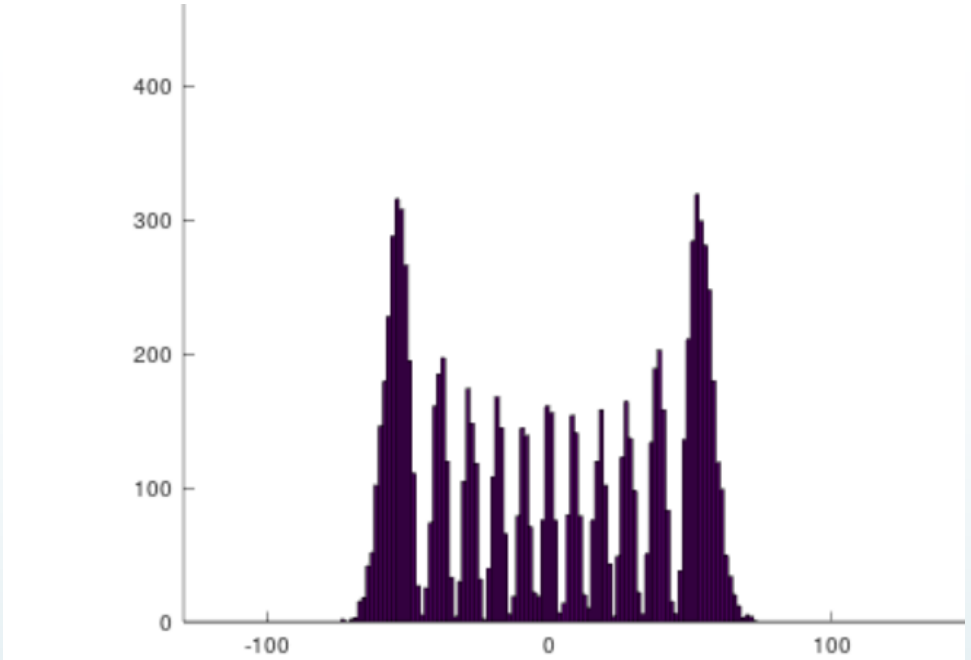
2. Include proper thermal distortions according to BE distribution

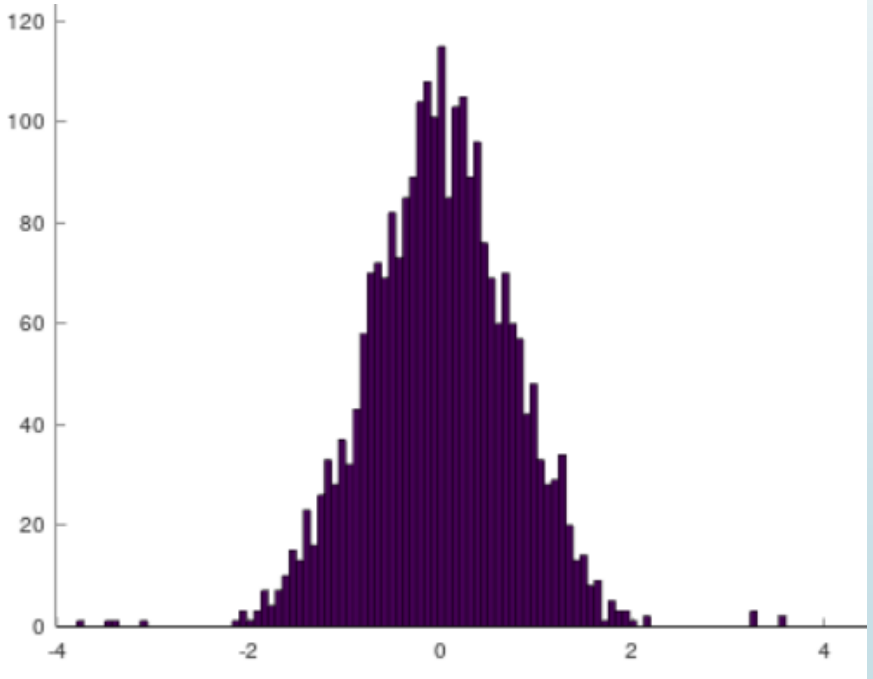
$$f(E) = \frac{1}{Ae^{E/kT} - 1}$$

Execute the Plan

3. Inverse Transform Sampling



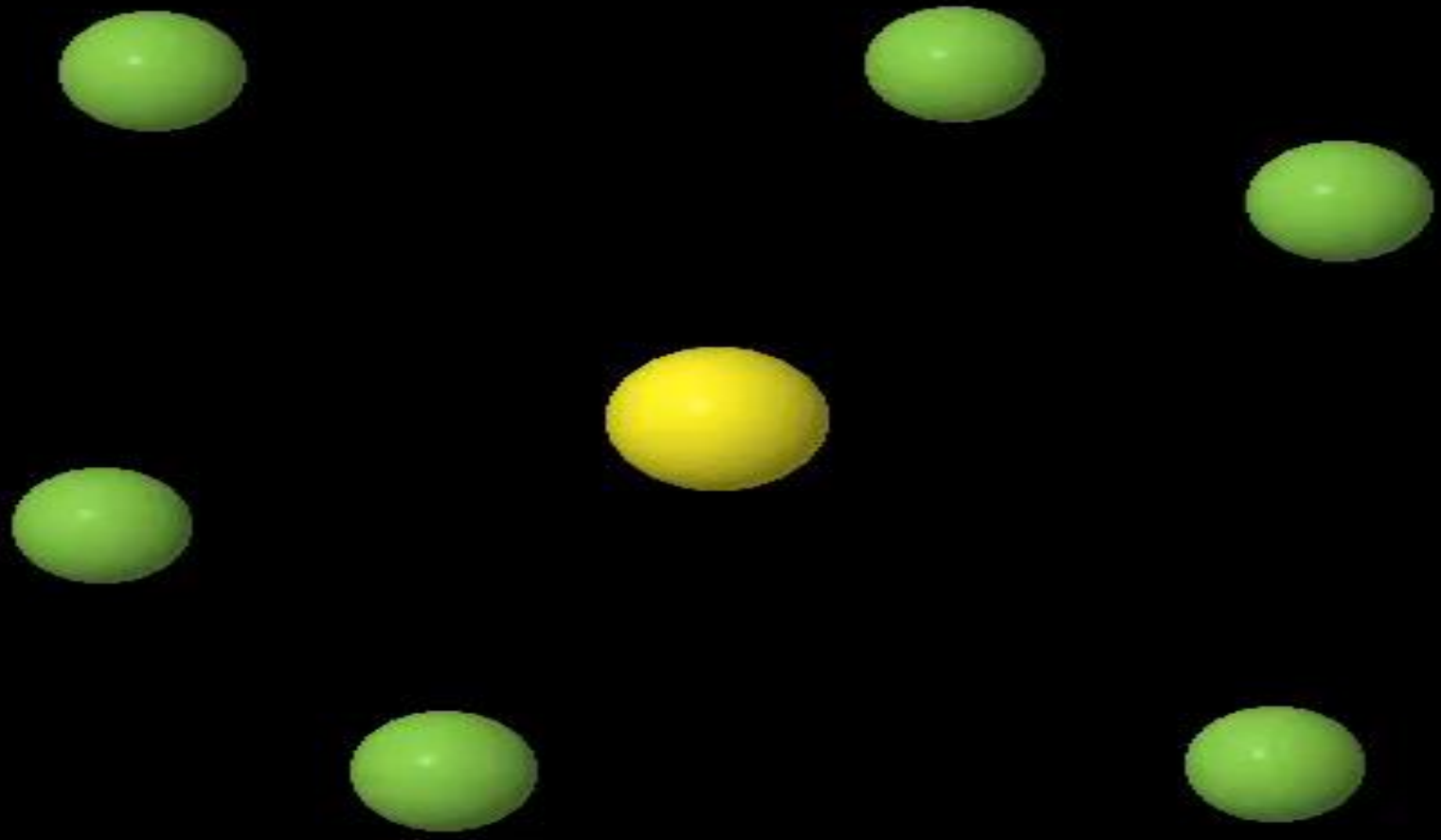




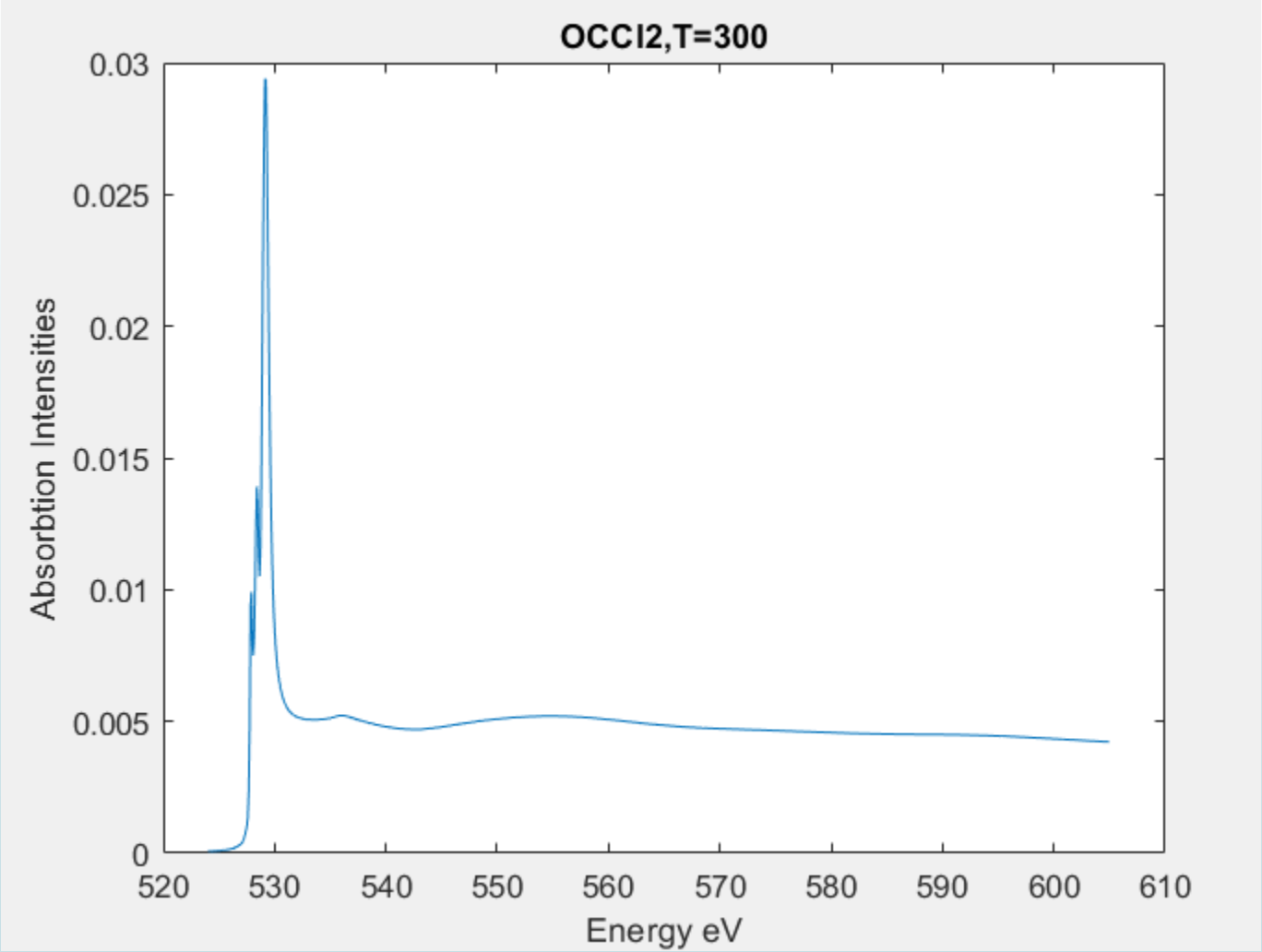
Generate Sampled Coordinates

- Use dynamical matrix of atoms to produce vibrational normal modes.
- Multiply generated amplitudes by displacement vectors
- Generate new coordinates.

1. 10.1103/PhysRevB.76.014301



Throw Away the Plan



Conclusion

PC: Meagan Sundstrom

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Questions