Extended X-Ray Absorptions Fine Structure Fitting using Genetic Algorithms

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Introduction

We have developed a machine learning related technique for automated analysis of Extended X-ray Absorption Fine Structure (EXAFS). It utilized a Genetic Algorithm (GA) to generate high quality fits of experimental spectra and used to uncover the local atomic structure:

(I) coordination numbers, (II) interatomic distances, and (III) lattice dynamics.

Genetic Algorithms

Genetic Algorithms (GA) was utilized to optimized the throughput and quality of the analysis. GA relies on using evolutionary operators to perform specific optimizations, such as mutation, crossover and fitness evaluation.

Verifications

- Copper K-edge at various temperature 10 (a), 50 (b), 150 (c) and 298 K (d)
  
  (a) 10K, \( \chi^2 = 0.323, R^2 = 0.942 \)
  
  (b) 50K, \( \chi^2 = 0.294, R^2 = 0.945 \)
  
  (c) 150K, \( \chi^2 = 0.130, R^2 = 0.960 \)
  
  (d) 298K, \( \chi^2 = 0.368, R^2 = 0.981 \)

- Atomic distance is very close to theoretical methods
- Debye-Waller factor (\( S^2 \)) increase due to Doppler broadening effect

Results

Operando Fitting

- Operando measurements leads to considerable amount of EXAFS data, enable variational changes in surface chemistry. We have applied similar techniques on Sn compounds in a lithium-ion battery.

Future Works

- Further reducing manual intervention
  - FEFF .inp as inputs using FEFF8.5L
  - Include self-adsorption correction
  - Coupled to material database such as Material Projects
  - Further constrains set on individual paths
  - Developing of Graphical User Interface
  - Utilizing similar algorithm to analysis X-ray photoemission (XPS)

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