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## structural transormations of photoswitchable complexes captured by quantitative XANES

structural transormations of photoswitchable complexes captured by quantitative XANES by LIU Xuanran

- 1. Introduction to XANES
- 2. Finite difference method

a) Finite Difference Method (FDM) and Green formalism

- b) multi-electronic extension using the "Time-Dependent DFT"
- c) Convolution with the FDMNES

3. Result of calcutaions for ground states of Febpy, Fedcpp and Fe-terpy: by using the coordinates of the molecule, we calculate the XANES by FDMNES and compared it to the experimental spectrums.

4. Simulation of the excited state by deformation of the molecule: we deform the molecule manually to simulate the reaction of the molecule when excited by the X-ray laser. And compared it to the experimental spectrum.

- 5. using of machine learning
- a) Approximation of XANES as a function of structural parameters
- b) Extra free method
- c) Quadratic refression
- d) Direct prediction of structure parameters from experimental XANES
- e) Extra free methods
- f) Convolutional neural networks

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Session Classification: Student session

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