MaMaSELF

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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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