P5567: XANES SPECTRA OF VANADIUM COMPLEXES CALCULATED BY TWO TDDFT METHODS

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- To extract the geometric and electronic structure information from experimental XANES spectra, we have used TDDFT methods to calculated the V K-edge spectra.
- The result shows V K-edge XANES can be calculated by LR-TDDFT and RT-TDDFT methods
- For LR-TDDFT calculation: the peaks (pre-edge and shoulder) assignment is very clear, especially the pre-edge peak can be quantitatively analysis by p-hybridization ratio
- For RT-TDDFT calculation: the obtained V k-edge XAENS agree with the experimental and LR-TDDFT calculation
- Future work

Extract the electronic information of RT-TDDFT calculated V K-edge XANES

Integrate treatment of relativistic effects