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RCMS Research Center for Materials Science, Nagoya University

Theoretical Chemistry Colloquium

June 19, 2013 (Wed), 14:00-15:30

RCMS, 2nd floor, Chemistry Gallery

Spectroscopic Calibration of Electronic Structure Theory: Basis Sets, Exchange and Correlation Functionals, Ground and Excited States

Prof. Dr. Robert K. Szilagyi
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Abstract: *The presentation will summarize our approach in using X-ray absorption spectroscopic results in defining the ground state electronic structure of transition metal complexes with unoccupied d-manifolds. The X-ray Absorption Near-Edge Spectral analysis (XANES) will be defined through a representative example of an Fe-S cluster, which is a biomimetic model of the catalytic center of FeFe-hydrogenase. The applicability of the methods will be extended to the metalloenzyme galactose oxidase that contains a Cu-O(Tyr-Cys) active site, several Cu/Ni containing non-innocent coordination complexes. The XANES data will be used for calibrating modern density functional theory and selecting the most reasonable basis set, exchange, and correlation functionals for the series of biomimetic Cu(II) complexes and then the complicated scenario of biological Fe-S clusters. The presentation will conclude by posing several challenges for parameterizing density functional tight binding method using XANES data.*

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