Joint Theory Seminar

European XFEL, CFEL & University of Hamburg

Thursday, 11 November 2021, 17:00 – 18:00

Dr. Niri Govind

Pacific Northwest National Laboratory, Richland, WA, USA

X-ray Spectroscopy Studies of Molecules and Materials with TDDFT-Based Approaches: Recent Applications and Developments

Over the last two decades, time-dependent density functional theory (TDDFT), in conjunction with suitable exchange-correlation functionals, has become a computationally attractive approach for studying excited-state spectra including X-ray spectra in a wide range of molecular and materials systems. In this talk, I will present our TDDFT-based developments and applications for X-ray spectroscopies with the open-source NWChem computational chemistry program. I will present recent work, where we have used the K-edge (Fe, O, N) XANES to study the transient species of the photoaquation reaction in aqueous ferrous hexacyanide, electron delocalization on the excited state in aqueous Fe(II)Ru(III), and ultrafast proton transfer. I will also cover recent work to model the L3-edge XANES of model Ru complexes. For the second part of our talk, I will present applications based on our valence-to-core (VtC) X-ray emission protocol (sulfur compounds, 3d and 4d transition metal systems). Finally, I will present our recent developments on resonant inelastic X-ray scattering (RIXS) calculations of transition metal complexes (2p4d RIXS of Ru model complexes) within a simplified linear-response TDDFT framework.

Suggested Papers:

1. Linear-Response and Real-Time Time-Dependent Density Functional Theory Studies of Core-Level Near Edge X-ray Absorption, K. Lopata, B.E. Van Kuiken, M. Khalil, N Govind, J. Chem. Theory Comput. 8, 9, 3284 (2012)
2. Simulating Valence-to-Core X-ray Emission Spectroscopy of Transition Metal Complexes with Time-Dependent Density Functional Theory, Y. Zhang, S. Mukamel, M. Khalil, N. Govind, J. Chem. Theory Comput, 11, 5804 (2015)
3. Comprehensive Experimental and Computational Spectroscopic Study of Hexacyanoferrate Complexes in Water: from the Infrared to X-ray Wavelengths, M. Ross, A. Andersen, Z. W. Fox, Y. Zhang, K. Hong, J-H. Lee, A. Cordones, A. M. March, G. Doumy, S. H. Southworth, M. A. Marcus, R. W. Schoenlein, S. Mukamel, N. Govind, M. Khalil, J. Phys. Chem. B, 122, 5075 (2018)
4. Elucidation of the Photoaquation Reaction Mechanism in Ferrous Hexacyanide using Synchrotron X-rays with Sub-Pulse-Duration Sensitivity, A. M. March, G. Doumy, A. Andersen, A. Al Haddad, Y. Kumagai, M-F. Tu, J. Bang, C. Bostedt, J. Uhlig, D. R. Nascimento, T. A. Assefa, Z. Nemeth, G. Vanko, W. Gawelda, N. Govind, L, Young, J. Chem. Phys, 151, 144306 (2019)
5. Probing Sulfur Chemical and Electronic Structure with Experimental Observation and Quantitative Theoretical Prediction of Kα and Valence-to-Core Kβ X-ray Emission Spectroscopy, W. M. Holden, E. P. Jahrman, N. Govind, G. T. Seidler, J. Phys. Chem. A, 124, 5415 (2020)
6. Valence-to-Core X-ray Emission Spectroscopy of Vanadium Oxide and Lithiated Vanadyl Phosphate Materials, E. P. Jahrman, W. H. Holden, N. Govind, J. J. Kas, J. Rana, L. F. J. Piper, C. Siu, M. S. Whittingham, T. T. Fister, G. T. Seidler, J. Materials. Chemistry A, 8, 32, 16332 (2020)
7. Resonant Inelastic X-ray Scattering Calculations of Transition Metal Complexes within a Simplified Time-Dependent Density Functional Theory Framework, D. R. Nascimento, E. Biasin, B. Poulter, M. Khalil, D. Sokaras, N. Govind, J. Chem. Theory Comput, 17, 5, 3031-3038 (2021)
8. Revealing the Bonding of Solvated Ru Complexes with Valence-to-Core Resonant Inelastic X-ray Scattering, E. Biasin, D. R. Nascimento, B. I. Poulter, B. Abraham, K. Kunnus, A. T. Garcia-Esparza, S. H. Nowak, T. Kroll, R. W. Schoenlein, R. Alonso-Mori, M. Khalil, N. Govind, D. Sokaras, Chemical Science, 12, 3713-3725 (2021)
9. Spectral Signatures of Ultrafast Excited State Intramolecular Proton Transfer from Computational Multi-edge Transient X-ray Absorption Spectroscopy, C.M. Loe, C. Liekhus-Schmaltz, N. Govind, M. Khalil, J. Phys. Chem. Letts (accepted and to appear shortly 2021)

Zoom link:

https://xfel.zoom.us/j/95235213686?pwd=Rm8xMU5Vcm1WR0pUa0hLNFpIZCthUT09

Meeting ID: 952 3521 3686

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