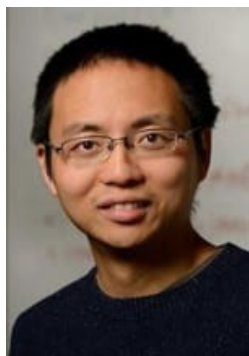


PHYSICAL CHEMISTRY SEMINAR



Prof. Lan Cheng

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Monday, Oct 18, 2021

4:00 PM

Young Hall 2033

“Relativity Throughout the Periodic Table: Scalar Relativity, Spin-Orbit Coupling, and Spin-Vibronic Interaction”



Special relativity plays an important role in heavy-element chemistry and is also relevant to calculations of light elements when aiming at high accuracy [1]. This presentation is focused on recent developments of relativistic quantum chemistry [2]. The applicability of relativistic quantum-chemical methods presented here is demonstrated with example applications, including vibronic branching ratios in lasercoolable molecules [3], x-ray spectroscopy involving elements across the periodic table [4], and spectra for molecules containing early actinides as examples for elements in the far reaches of the periodic table [5].

[1] P. Pyykko "Relativistic Effects in Structural Chemistry." *Chem. Rev.* 88, 563-594 (1988).

[2] J. Liu and L. Cheng "Relativistic Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods." *WIREs Mol. Sci.* e1536, <https://doi.org/10.1002/wcms.1536> (2021).

[3] C. Zhang, B. L. Augenbraun, Z. D. Lasner, N. B. Vilas, J. M. Doyle, and L. Cheng "Accurate prediction and measurement of vibronic branching ratios for laser cooling polyatomic molecules." in revision (2021) arXiv:2105.10760.

[4] S. H. Southworth, R. W. Dunford, D. Ray, E. P. Kanter, G. Doumy, A. M. March, P. J. Ho, B. Krassig, Y. Gao, C. S. Lehmann, A. Picon, L. Young, D. A. Walko, L. Cheng "Observing pre-edge Kshell resonances in Kr, Xe, and XeF₂." *Phys. Rev. A* 100, 022507 (2019).

[5] M. Marshall, Z. Zhu, J. Liu, L. Cheng, and K. H. Bowen "Photoelectron Spectroscopic and ab initio Computational Studies of the Anion, HThO⁻." *J. Phys. Chem. A* 125, 1903-1909 (2021).