

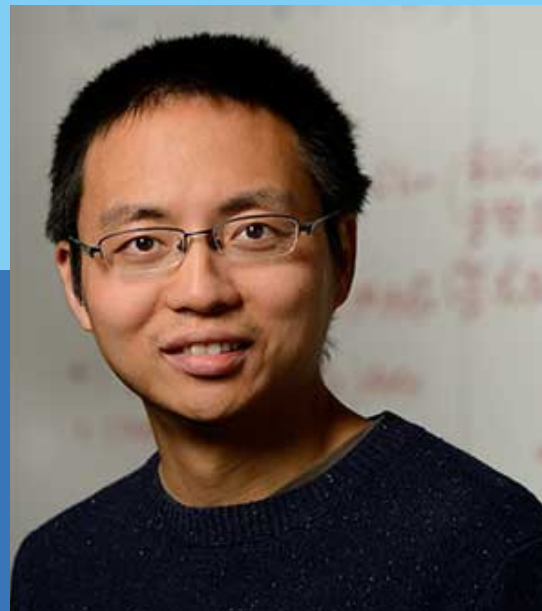
PHYSICAL CHEMISTRY SEMINAR

Tuesday, February 22, 2022

11:00 a.m. (CT)

Learning Studio, Room 1435

Host: Prof. Yang Yang



Extending Accurate Quantum Chemistry to Heavy Elements

Professor Lan Cheng
Johns Hopkins University

The presentation is focused on recent development of relativistic exact two component wave function-based methods. An atomic mean-field spin-orbit approach within exact two-component theory, the X2CAMF scheme, is shown to significantly enhance the computational efficiency while retaining the accuracy of the parent four component Dirac-Coulomb-Breit approach for calculations of many molecular properties. An efficient implementation of the X2CAMF scheme together with analytic energy gradients for spin-orbit coupled-cluster methods enables accurate calculations of geometries and properties for molecules containing heavy atoms. The applicability of these relativistic quantum-chemical methods is demonstrated using example applications to x-ray spectroscopy and heavy-element spectroscopy pertinent to laser cooling of molecules.



Department of Chemistry

UNIVERSITY OF WISCONSIN-MADISON

For more information, contact Alisa Gradney at agradney@wisc.edu