ABSTRACT: The Molecular Sciences Software Institute (MolSSI) is a nexus for research, education, and cooperation serving the worldwide community of computational molecular scientists - a broad field including of biomolecular simulation, quantum chemistry, and materials science. The Institute focuses on the software infrastructure, education, standards, and best-practices that are needed to enable the molecular science community to open new windows on the next generation of scientific Grand Challenges, ranging from the simulation of intrinsically disordered proteins associated with a range of diseases to the design of new catalysts vital to the global chemical industry and climate change. The MolSSI is working to enable the computational molecular sciences community to work together to leverage its diverse capabilities that will reduce or eliminate the gulf that currently delays by years the practical realization of theoretical innovations. Ultimately, the Institute will enable computational scientists to tackle problems that are orders of magnitude larger and more complex than those currently within our grasp. This lecture will provide an overview of the Institute’s activities, goals, and vision.

SHORT BIO: Dr. Ben Pritchard earned his B.S. in general chemistry from the Rochester Institute of Technology (RIT). During his studies there, he also worked as an analytical chemist at Xerox Corp. After graduating from RIT, he joined the research group of Dr. Jochen Autschbach at the University at Buffalo, where his graduate research largely focused on computation of paramagnetic nuclear magnetic resonance (NMR) using density functional theory. Throughout his undergraduate and graduate careers, Ben was an avid hobbyist programmer, starting and abandoning many projects, including an ill-fated attempt at a linux-like package manager for Windows and an ncurses interface for PBS/Torque. The skills from these projects were, however, put to good use as a postdoc, both in developing a density-fitting library (PANACHE) while at Virginia Tech with MolSSI Director, Prof. Daniel Crawford, and in developing a vectorized electron-repulsion integral library (simint) at Georgia Tech under Prof. Edmond Chow. Ben has a passion for programming, with a particular focus on C++, Python, and how a marriage of the two can used in forming coherent frameworks in computational chemistry. Other current interests are in computation of molecular integrals, in terms of both optimizing for performance, and in determining the accuracy of common algorithms and implementations.

Monday, March 26, 2018
11:00 am - 12:00 Noon in NSC 306