CHEM 5914 Literature Review and Research Plan – COVER SHEET – Fall 2017

Student's Name	**Karl Pierce**
Review Title	Tensor Reduced Explicitly Correlated Electronic Structure Methods
Student's Email Address	Kmp5@vt.edu
Date Submitted	08/30/17
Response Deadline	9/10/17

Check the correct box. (In MS Word double-click on box and change "default value")

☒	**Outline**. Submit to the Research Director only by September 1st. Respond within 1 week.
☐	**Preliminary Draft**. Submit to Research Director only by September 29th. Response needed by Friday, October 13.
☐	**First Draft**. Submit to Advisory Committee by October 31st. Responses needed by Monday, November 13.
☐	**Final Draft**. Submit to Advisory Committee by December 1st. Responses needed Monday of Exam Week.

List your ENTIRE Advisory Committee here:

Function	Name	Department	Email
Chair	Edward Valeev	CHEM	valeev76@vt.edu
Co-Chair (if you have one)			
Member	T. Daniel Crawford	CHEM	crawdad@vt.edu
Member	Nicholas Mayhall	CHEM	nmayhall@vt.edu
Member	Diego Troya	CHEM	troya@vt.edu
Member			

Honor Pledge. Turning in any document for CHEM 5914 constitutes a pledge to conform to the policies and procedures of the Virginia Tech Graduate Honor System.

Faculty Instructions are available on the CHEM Grad Program Scholar site in the Literature Review folder.

Literature Review Outline

- Introduction
- Ab Initio Many Body Quantum Mechanics
  I. Hartree Fock
  II. Electronic Correlation
    - Many body perturbation theory
    - Configuration interaction theory
    - Couple cluster theory
  III. Explicitly Correlated Methods
    - Motivation
    - Explicitly correlated many body perturbation theory
    - Explicitly correlated couple cluster methods
- Tensor Algebra Methods to reduce Computational Complexity in Quantum Chemistry
  I. Tensor Reduction methods in a Canonical Quantum Chemistry Framework
    - Density fitting/resolution of the identity
    - Pair natural orbitals/pair atomic orbitals
    - Tensor decomposition methods
      * Tensor hypercontraction
      * Cholesky decomposition
      * Canonical product
      * Tucker decomposition
  II. Tensor Ansätze to Schrödinger like Equations
    - Motivation for these kinds of methods (MPS, TNS, TTNS, DMRG etc) How this section is different from the "Canonical QC" section.
- Research Plan