NSERC/DURA Opportunity for Summer 2021 with Prof. Marko Horbatsch

**Computer Simulation of Small Molecules**

The development of a computer program to calculate properties of small molecules using a linearly combined atomic orbital (LCAO) method. The idea is to start with existing orbitals for atoms which are constituents for a given molecule (e.g., MgF, i.e., magnesium monofluoride) using archived self-consistent field solutions. Using ideas from density functional theory an effective one-electron model will be developed to describe the ground state of the molecule and its low-lying excited electronic levels (initially neglecting spin-orbit coupling).

Prerequisites for this work: completion of PHYS3040 Modern Physics with an excellent grade, and some computing experience (in at least one of: Mathematica, Fortran, Python, or Matlab).