

# Constrained Unrestricted Hartree Fock and Single Excitation Configuration Interaction

**Ruben Van der Stichelen**

$$\langle \mathbf{G} | \mathbf{QC} | \mathbf{G} \rangle$$

Ghent University  
April 16, 2021

- 1 Introduction
- 2 Constrained Unrestricted Hartree Fock Theory
  - 2.1 Theory
  - 2.2 Implementation
  - 2.3 Results
- 3 Single Excitation Configuration Interaction
  - 3.1 Theory
  - 3.2 Implementation
- 4 The CUHF Wave Function in the CIS Approach
- 5 Applications