

Chad Cronce

SCARP

Presentation date: Wed. July 29<sup>th</sup>

### Using EOMCC to calculate the energies of excited state diatomic molecules

Calculating the energies of molecules is important as it can give insight to their properties and their role within a reaction. The energy for an atom or molecule can be found by solving the Schrödinger equation directly, though this has only been done in full for the hydrogen atom. For larger atoms, or molecules, approximations need to be assumed for a solution to be found. The first, and most crude, approximation is called Hartree-Fock which assumes that the wave function for an electron can be estimated by a Slater determinant. The wave function of an electron is the equation that describes how the electron behaves within any given region of space. Although this is the crudest approximation, the results are comparable to experimental results within reason. Further improvements have been made essentially extending from this approximation. Basis sets have been added to further define the region of space that the electron can exist in, to allow for further accuracy. A method was adapted to vary the Slater determinant to give the most accurate energy possible. Further computational methods first use the Hartree-Fock method to get an approximated wave function, and will continue to vary other parameters to achieve a better energy. Couple cluster methods do this and use an approximation for the equation of motion of an electron within the molecule to obtain better results for the ground state energy of the molecule. The equations used also have several properties that allow them to estimate the energy of dimers or higher congregates to find the energy of the monomer. Also, these equations allow for the outcome of the energy of several excited states, to a relatively high degree of accuracy. This is important as not many of the methods that are used for electronic structure calculations have the ability to predict the energies of excited states.

It is hoped that this will allow for the study of reactions in a better way due to the ability to correctly calculate the energies of some intermediates within reactions where molecules go through excited states, especially if these excited states have not been clearly studied. Therefore, a comparison of the ground state energy using this method and others will be conducted on a simple diatomic molecule. Once completed, the first several excited states will then be analyzed and compared to literature values. If time permits, a comprehensive analysis can be done to predict rotational and vibrational constants and excitations, even leading to theoretical spectra of possible transitions that may occur from the ground state into these higher excited states.