

DESCRIPTION FOR THE GENERAL PUBLIC

In a recent years there has been a renewed interest in small molecular system which are intensively studies in several fields of science at the border of chemistry and physics, *e.g.*, astrochemistry or ultracold molecular physics. A large fraction of the experimental techniques used in the aforementioned studies require a comprehensive theoretical support. In many cases knowledge of, *e.g.*, molecular geometry, harmonic frequencies, relative energies is necessary in advance. Additionally, these theoretical calculations performed with quantum chemistry methods need to be of good quality, so that design and faithful interpretation of the experiments is possible.

Nearly all quantum chemical calculations are based on the concept of the basis set which defines the space used to search for an approximate wavefunction. As a result, the choice of the type and size of the basis set is crucial for the accuracy of the solution. The basis set of Slater-type orbitals appears to be the natural basis set for the quantum chemical calculations. It has many advantages compared to the other widely used basis sets and asserts, *e.g.*, the correct behaviour of the wavefunction when an electron is close to the nuclei. Unfortunately, the applicability of Slater-type orbitals has been greatly hampered thus far, mainly by the difficulties in the evaluation of the molecular integrals.

The main goal of this project is to make the first step towards application of the Slater-type orbitals to the aforementioned calculations. The starting point for the proposed method are the techniques developed by us for the diatomic systems. We put forward their generalisation which allows to apply new schemes also for larger systems. Additionally, we propose a set of other tweaks and improvements which contribute to algorithms of much greater generality and reliability. Finally, this leads to a significant increase in the quality of the theoretical predictions and facilitates the cooperation at the border of theory and experiment.