The modern, quantum-chemical picture of atoms and molecules is based on an equation devised in the 1920s, the Shröedinger equation, which yet defied exact solution for general systems of more than two electrons. Because the most important chemical systems include at least tens of electrons, the description of these systems is difficult and requires ingenuity.

Because each electron influences all the other electrons, a computational chemist doing a simulation using her computer needs to describe Coulomb interactions within each pair of electrons in their instantaneous positions. This problem is known in quantum chemistry as electron correlation. Numerous methods for approximate description of this interaction has been proposed since the beginning of quantum chemistry. This problem is still a great challenge – high accuracy methods are so costly that can be applied only to small systems, whereas cheap methods are too inaccurate to be useful.

Apart from the electric charge, electrons as elementary particles possess an intrinsic property called spin. Spin can interact with the motion of an electron through the so-called spin-orbit interaction. The spin-orbit interaction has influence on many chemical properties, such as splitting of energy levels, existence of forbidden transitions, and phosphorescence. Currently, a few theoretical methods exist which can describe spin-orbit interactions while simultaneously accounting for electron correlation. Some of these methods fail to satisfy important physical conditions, others cannot be applied routinely. The work proposed in this Project will be the first available computational method free of these issues.