This thesis focuses on the three pillars of any high-precision *ab initio* calculation: on the Hartree-Fock (HF) model, on the choice of a suitable basis set, and on the inclusion of electron correlation.

We start with a study of singular properties of the HF model. Specifically, we systematically investigate the stability of all atomic closed-shell systems up to xenon using a symmetry-adapted Thouless stability matrix. To obtain a global view on the stability of a particular isoelectronic sequence, we employ high-order perturbative method and then analyze the obtained series. This allows us to determine onsets of spin and orbital symmetry breaking. In addition, we also propose a physical meaning of the instabilities.

In the next part of this thesis, we focus on the use of the Sturmian basis set for relativistic calculations. We propose a numerically stable algorithm for the evaluation of one- and two-electron matrix elements. Thus we defeat the major impediment of a wider use of this basis set in precise atomic structure calculations. The use of the proposed method and its significance is illustrated on a series of calculations. For instance, we evaluate the so-called parity non-conserving amplitude for cesium; this is a second-order property and thus greatly depends on the accuracy of the used wave functions.

The last part of this thesis deals with the inclusion of electron correlation. We use the well-known coupled cluster (CC) method for closed shells and a combined configuration interaction-CC (CI-CC) method for one-electron open shells. We take advantage of the spherical symmetry of atoms and propose a symmetry-adapted form of the CC and CI-CC approaches; this idea significantly reduces the number of terms to be evaluated as well as the number of equations to be solved. This method is illustrated on the ionization energies of I.A elements.