Obviating the need for costly experimental measurements, computer simulations greatly facilitate uncovering diverse properties of Coulombic systems (i.e. atoms, molecules, polymers, and crystals). For this reason, progress in material science and drug design is becoming increasingly dependent on the availability of numerical methods that, in order to be competitive with experimental approaches, have to be both sufficiently accurate and computationally inexpensive.

Quantum chemistry has a whole lot of such numerical methods at its disposal. The core quantity in most of these methods is the so-called electronic wavefunction that fully describes any property of a given system. This wavefunction is a complicated mathematical object dependent on the coordinates of all electrons. Its complexity has prompted quantum chemists to seek alternative descriptions of Coulobic systems in terms of simpler quantities that are more amenable to calculation and interpretation. One of such quantities is the one-electron density whose simple dependence on three Cartesian coordinates and electron spin has been the primary reason for its widespread use in electronic structure theory.

Many types of interactions between atoms and molecules (e.g. covalent bonds and London forces) are inherently two-electron phenomena, in which the electron correlation plays an important role. Traditionally, chemical bonding is described with one-electron quantities (such as orbitals and the one-electron density) whereas the extent of electron correlation is quantified with various indices. Since this separate treatment of those two closely intertwined phenomena is artificial and counter-intuitive, alternative approaches are needed. The most natural choice for the core quantity in these approaches is the two-electron density. Unfortunately, properties of the two-electron density are much less known than those of its one-electron counterpart.

In this grant proposal, a comprehensible research program aiming at the rectification of this undesirable situation is described. New concepts, such as densitals and ditopology, are introduced in order to aid characterization of atomic and molecular two-electron densities whose computation is expected to become more accurate with new numerical techniques such as double Drachmanization. When completed, the proposed research will open the avenue to faster and more accurate numerical simulations benefiting not only scientists but, thanks to accelerated development of new medicines and materials, also people of all walks of life.