Progress in material science and drug design is becoming increasingly dependent on the availability of numerical simulations that make it possible to obtain information about properties of atoms, molecules, polymers, and crystals without resorting to costly experimental measurements. In order to be competitive, such simulations, also known as molecular modeling, have to be both sufficiently accurate and computationally inexpensive. Quantum chemistry has a whole lot of such numerical methods at its disposal. However, despite over half a century of sustained improvements, these methods are still too expensive to be of use for very large systems that are often encountered in practical research.

There is one family of quantum-chemical methods collectively known as functional theory. Its most popular incarnation, namely DFT (density functional theory) allows for relatively inexpensive calculations that, however, often want for accuracy of their results. For this reason, there has been recent resurgence of research on alternative formalisms involving functionals. Among them, the 1-matrix (a.k.a. one-electron reduced density matrix or simply density matrix) functional theory (DMFT) appears to be the most promising one.

In this grant proposal, we describe ways of improving the accuracy of DMFT and extending its applicability envelope. A broad spectrum of investigations that aim at achieving this end is put forward, ranging from purely mathematical approaches to numerical testing. When completed, the proposed research will open the avenue to faster and more accurate molecular modeling that will benefit not only scientists but, by speeding up development of new medicines and materials, also people of all walks of life.