The ground-state energy of an atom or molecule as well as all of its one- and two-electron properties can be computed from the ground-state two-electron reduced density matrix (2-RDM). While the significance of the 2-RDM was recognized in the mid-1950s, a direct calculation of the 2-RDM without the wave function was impeded for many years by the need to constrain the 2-RDM to derive from an $N$-electron wave function. These constraints became known as $N$-representability conditions. Two general approaches to the direct calculation of the 2-RDM for many-electron atoms and molecules have recently emerged: (i) the variational calculation of the 2-RDM subject to $N$-representability constraints known as positivity conditions, and (ii) the non-variational calculation of the 2-RDM from solving the anti-Hermitian contracted Schrödinger equation. These two approaches will be discussed with special emphasis on the most recent advances in the variational 2-RDM method.


