natural population analysis (NPA)

The analysis of the electron density distribution in a molecular system based on the orthonormal natural atomic orbitals. Natural populations, $n_i(A)$ are the occupancies of the natural atomic orbitals. These rigorously satisfy the Pauli exclusion principle: $0 < n_i(A) < 2$. The population of an atom $n(A)$ is the sum of natural populations $n(A) = \sum_A n_i(A)$. A distinguished feature of the NPA method is that it largely resolves the basis set dependence problem encountered in the Mulliken population analysis method.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1954