

### **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

$$n(A) = \sum n_i(A).$$

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.

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