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natural bond orbital (NBO)

The orbital which is formed from natural hybrid orbitals. For a localized σ-bond between atoms A and B, the NBO is:

$$\sigma_{AB} = c_A\, h_A + c_B\, h_B$$

where h_A and h_B are the natural hybrids centred on atoms A and B. NBOs closely correspond to the picture of localized bonds and lone pairs as basic units of molecular structure, so that is possible to conveniently interpret *ab initio* wave-functions in terms of the classical Lewis structure concepts by transforming these functions to NBO form.

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

