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