

**natural bond orbital (NBO)**

The orbital which is formed from natural hybrid orbitals. For a localized  $\sigma$ -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.

1999, 71, 1954