extended Hückel MO method (EHMO)

A semi-empirical all-valence electron quantum mechanical method which uses the same approximations, apart from π-approximation and neglect of overlap integrals, as those of the Hückel molecular orbital theory. The method reproduces relatively well the shapes and the order of energy levels of molecular orbitals. The account for overlap makes it possible to describe the net destabilization caused by interaction of two doubly occupied orbitals, which effect is not reproduced by HMO theory.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1939