Koopmans' theorem

Directly relates experimental ionization potentials with energy levels of molecular orbitals. The theorem states that the ionization potential required to remove an electron from the orbital Ψ_i is given by the negative value of the energy of the orbital, $-\varepsilon_i$, as calculated within the Hartree–Fock approximation. The theorem is not applied to localized molecular orbitals, which are not eigenfunctions of the effective hamiltonian.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1949