Born - Oppenheimer (BO) approximation

Representation of the complete wave-function as a product of an electronic and a nuclear part

$$\Psi (r,R) = \Psi_e (r,R)\Psi_N(R)$$

where the two wave-functions may be determined separately by solving two different Schroedinger equations. The validity of the Born-Oppenheimer approximation is founded on the fact that the ratio of electronic to nuclear mass ($m/M \cong 5 \times 10^{-4}$) is sufficiently small and the nuclei, as compared to the rapidly moving electrons, appear to be fixed. The approximation breaks down near a point where two electronic states acquire the same energy (see Jahn-Teller effect). The BO approximation is often considered as being synonymous with the adiabatic approximation. More precisely, the latter term denotes the case when Ψ_e diagonalize the electronic Hamiltonian. Thus, the adiabatic approximation is an application of the BO approximation.

1999, *71*, 1929