



Configuration Interaction

By Frederic P. Miller

Alphascript Publishing. Taschenbuch. Condition: Neu. Neuware - Configuration interaction (CI) is a post-Hartree Fock linear variational method for solving the nonrelativistic Schrödinger equation within the Born Oppenheimer approximation for a quantum chemical multi-electron system. Two meanings are connected to the term configuration interaction in this context. Mathematically, configuration simply describes the linear combination of Slater determinants used for the wave function. In terms of a specification of orbital occupation (for instance, $(1s)^2(2s)^2(2p)^1$), interaction means the mixing (interaction) of different electronic configurations (states). Due to the long CPU time and immense hardware required for CI calculations, the method is limited to relatively small systems. 76 pp. Englisch.



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