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In computational physics and chemistry, the Hartree-Fock (HF) method is a method of approximation for the determination of the wave function and the energy of a quantum many-body system in a stationary state.. The Hartree-Fock method often assumes that the exact, N-body wave function of the system can be approximated by a single Slater determinant (in the case where the particles are ...

Hartree-Fock method - Wikipedia

Although the mathematical basis of quantum chemistry had been laid by Schrödinger in 1926, it is generally accepted that the first true calculation in quantum chemistry was that of the German physicists Walter Heitler and Fritz London on the hydrogen (H_2) molecule in 1927. [citation needed] Heitler and London's method was extended by the American theoretical physicist John C. Slater and the ...

Quantum chemistry - Wikipedia

Insights from spectroscopic experiments led to the development of quantum mechanics as the common theoretical framework for describing the physical and chemical properties of atoms, molecules and ...

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