

A brief history of *ab-initio* calculation of electronic systems

Jinyuan Wu

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1 Orbitals

From Wiki:

Lothar Meyer in his 1864 book, *Die modernen Theorien der Chemie*, contained an early version of the periodic table containing 28 element

In 1916, G. N. Lewis proposed that a chemical bond forms by the interaction of two shared bonding electrons, with the representation of molecules as Lewis structures. The chemist Charles Rugeley Bury suggested in 1921 that eight and eighteen electrons in a shell form stable configurations

However, for hydrogen alone, in 1927 the Heitler–London theory was formulated which for the first time enabled the calculation of bonding properties of the hydrogen molecule H_2 based on quantum mechanical considerations.

2 Density functional theories

<https://www.birs.ca/workshops/2019/19w5035/files/Cances.pdf>