

Ab initio quantum chemistry methods

***Ab initio* quantum chemistry methods** are computational chemistry methods based on quantum chemistry.^[1] The term *ab initio* was first used in quantum chemistry by **Robert Parr** and coworkers, including **David Craig** in a semiempirical study on the excited states of benzene.^{[2][3]} The background is described by Parr.^[4] *Ab initio* means "from first principles" or "from the beginning", implying that the only inputs into an *ab initio* calculation are physical constants.^[5] *Ab initio* quantum chemistry methods attempt to solve the electronic Schrödinger equation given the positions of the nuclei and the number of electrons in order to yield useful information such as electron densities, energies and other properties of the system. The ability to run these calculations has enabled theoretical chemists to solve a range of problems and their importance is highlighted by the awarding of the Nobel prize to John Pople and Walter Kohn.^[6]

Accuracy and scaling

Ab initio electronic structure methods aim to calculate the many electron function which is the solution of the non-relativistic electronic Schrödinger equation (in the Born–Oppenheimer approximation). The many electron function is generally a linear

Ab Initio Methods In Quantum Chemistry I

Patrick Cassam-Chenai



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