Quantum mechanical chemistry dates back to the late 1920's when the hydrogen bond was first identified as a significant force in chemistry. This quantum mechanical approach was initially developed to explain the stability of molecules and to predict their properties. However, the mathematical framework of quantum mechanics, embodied in Schrödinger's equation, is not always tractable for realistic molecules. While there are many numerical methods for solving this equation, there are no exact solutions to it for anything more complicated than the hydrogen molecule.

The development of computational methods in the 1950's, the development of density functional theory in the 1970's, and the increasing availability and speed of computers in the 1980's, have catalyzed a quantum mechanical renaissance which resulted in molecular associations via hydrogen bonds. Such electrostatic effects contribute significantly to the macroscopic properties of matter.

These advances catalyzed this progress:
- the development of computational methods by John Pople and many others in the 1950’s
- the development of density functional theory by Walter Kohn and others, and
- the increasing availability and speed of computers.

Electron density increases toward the nuclei of a molecule. To illustrate this, a second isosurface of electron density is given in Figure 6. The distance between the inner and the outer electron density isosurfaces differs for different atoms. It is larger for the chlorine atoms and smaller for the fluorine atoms.

Bond lengths, angles, and atomic radii used to describe the molecular structure of the methane molecule. To illustrate this, a second isosurface of electron density is given in Figure 6. The distance between the inner and the outer electron density isosurfaces differs for different atoms. It is larger for the chlorine atoms and smaller for the fluorine atoms.

Electrostatic potential describes the interaction energy of a positive probe at each point around a molecule. It is color-mapped on the electron density isosurfaces.

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Electrostatic potential describes the interaction energy of a positive probe at each point around a molecule. It is color-mapped on the electron density isosurfaces. Blue marks electron-poor regions while red indicates electron-rich regions. Fluorine atoms are centers of negative charge. Non-uniform charge distribution results in molecular associations via hydrogen bonds.

Another important result of ab initio calculations is the charge distribution in a molecule. This is color-mapped on the electron density isosurfaces. Blue marks electron-poor regions while red indicates electron-rich regions. Fluorine atoms are centers of negative charge. Non-uniform charge distribution results in molecular associations via hydrogen bonds.