Abderrezak Torche | 11.05.2023

New types of chemical bonds

The concept of electrons sharing to form molecules from independent atoms is one of the most fascinating aspects of quantum mechanics. For many years, chemical bonds were classified into three categories: covalent, non-covalent, and ionic, according to the seminal work of Pauling [JACS **1931**, *53*, 3225]. However, recent studies have shown that exceptions to these categories are possible.

THE NATURE OF THE CHEMICAL BOND.
II. THE ONE-ELECTRON BOND AND THE THREE-ELECTRON BOND

By Linus Pauling

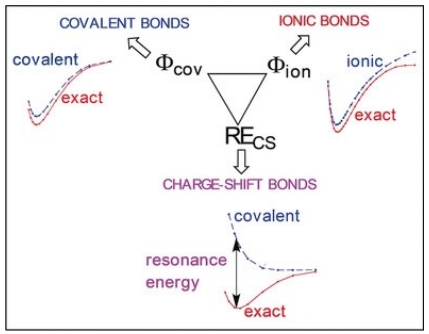
Received June 11, 1931 Published September 5, 1931

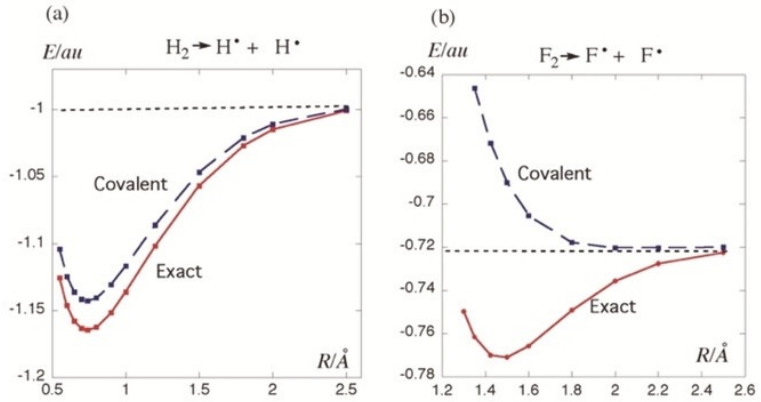
Here, I explore three types of non-standard chemical bonding where the ground state energy cannot be determined by simply minimizing the energy of the shared molecular orbitals.

Charge-shift bonding

In covalent and ionic bonds, the bond energy is dominated by the respective structures (covalent or ionic). In charge-shift bonds, the bonding is dominated by the covalent-ionic resonance energy, while the primary structure may even be repulsive.

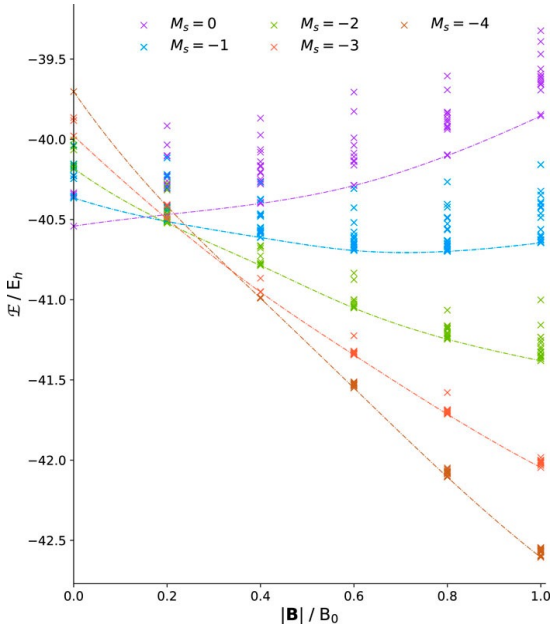
The electronic origin of this type of bond is the resonant mixture of covalent and ionic character. It is the shared change-density and its fluctuation that ensures in the same time both the covalent ionic character of the bond





Paramagnetic Bonding

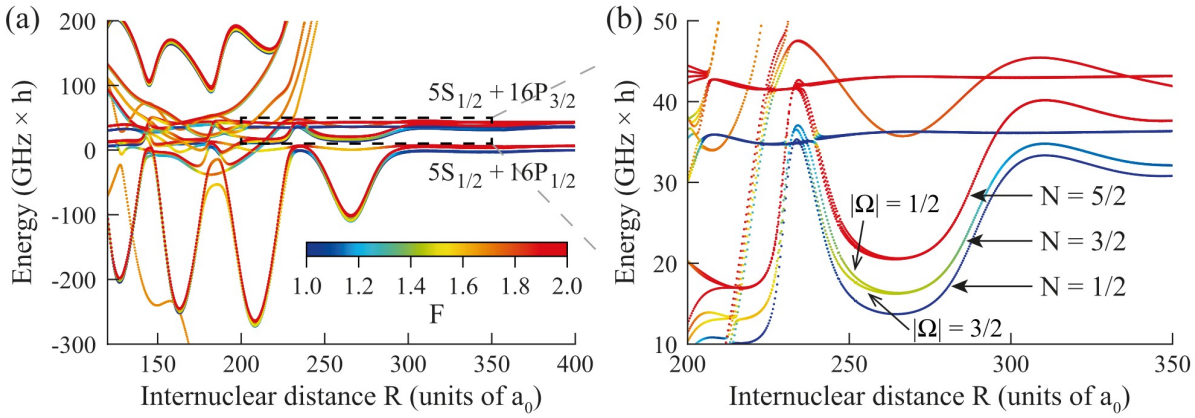
In strong magnetic fields, such as those present in the atmospheres of white dwarfs (on the order of 10^5 T) and other stellar objects, FCI computations suggest that H_2 molecule is stabilized in the antibonding triplet state rather than the singlet states and adopts a preferred perpendicular orientation.



Science **2012**, *337*, 327.

Ultralong-range Rydberg molecules interaction

This bonding is ensured via multipole forces to form Rydberg–Rydberg molecules with very large internuclear distances up to 50-100 nm. Note the ultra-low binding energy.



Nature **2009**, *458*, 1005.