

CHAPTER OVERVIEW

27: The Chemical Bond in Diatomic Molecules

In this chapter we will see a couple of examples of how the concept and mathematics of quantum mechanics can be applied to understand the chemical bond in molecules. We will start from the simplest molecule, the H_2^+ molecular ion, and then we will move on to the simplest two-electron bond in the hydrogen molecule. To simplify the notation in this chapter, we will move away from S.I. units and use a set tailored for molecules, called *atomic units (a.u.)*. This set of units is built by setting $\hbar = e = m_e = a_0 = 1$. As an example of the simplification that a.u. allows, the energy eigenvalues of the hydrogen atom, Equation 21.8, simply becomes $E_n = -\frac{1}{2n^2}$ in the a.u. of energy, which are called Hartrees.

[27.1: The Chemical Bond in the Hydrogen Molecular Cation](#)

[27.2: The Chemical Bond in the Hydrogen Molecule](#)

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