

### 3.1: The Covalent Bond and Quantum Mechanics

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The behavior of electrons in molecules and atoms is described by quantum mechanics; classical (Newtonian) mechanics cannot be used because the de Broglie wavelengths ( $\lambda=h/mv$ ) of the electrons are comparable with molecular (and atomic) dimensions.

The relevant quantum-mechanical ideas are as follows:

- Electrons are characterized by their entire distributions (called wave functions or orbitals) rather than by instantaneous positions and velocities: an electron may be considered always to be (with appropriate probability) at all points of its distribution (which does not vary with time).
- The kinetic energy of an electron decreases as the volume occupied by the bulk of its distribution increases, so delocalization lowers its kinetic energy.

$$KE = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} \approx \frac{A}{D^2} \approx \frac{A}{V^{\frac{2}{3}}}$$

- The potential energy of interaction between an electron and other charges is as calculated by classical physics, using the appropriate distribution (wave function) for the electron: an electron distribution is therefore attracted by nuclei and its potential energy decreases as the average electron-nuclear distance decreases.

$$PE \approx -\frac{B}{D} \approx -\frac{B}{V^{\frac{1}{3}}}$$

- A minimum-energy electron distribution represents the best compromise between concentration near the nuclei (to reduce potential energy) and delocalization (to reduce kinetic energy).

$$E \approx KE + PE \approx \frac{A}{V^{\frac{2}{3}}} - \frac{B}{V^{\frac{1}{3}}}$$

A bond will form between two atoms when the electron distribution of the combined atoms (molecular orbital) yields a significantly lower energy than the separate-atom distributions (atomic orbitals). An example is a covalent bond, in which two electrons, one originally on each atom, change their distributions so that each extends over both atoms.

\*Taken from "Molecules" in The Encyclopedia of Physics by Frank E. Harris (with some additions and modifications by Frank Rioux)

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