Quantum Mechanical Approaches to Molecular Bonding

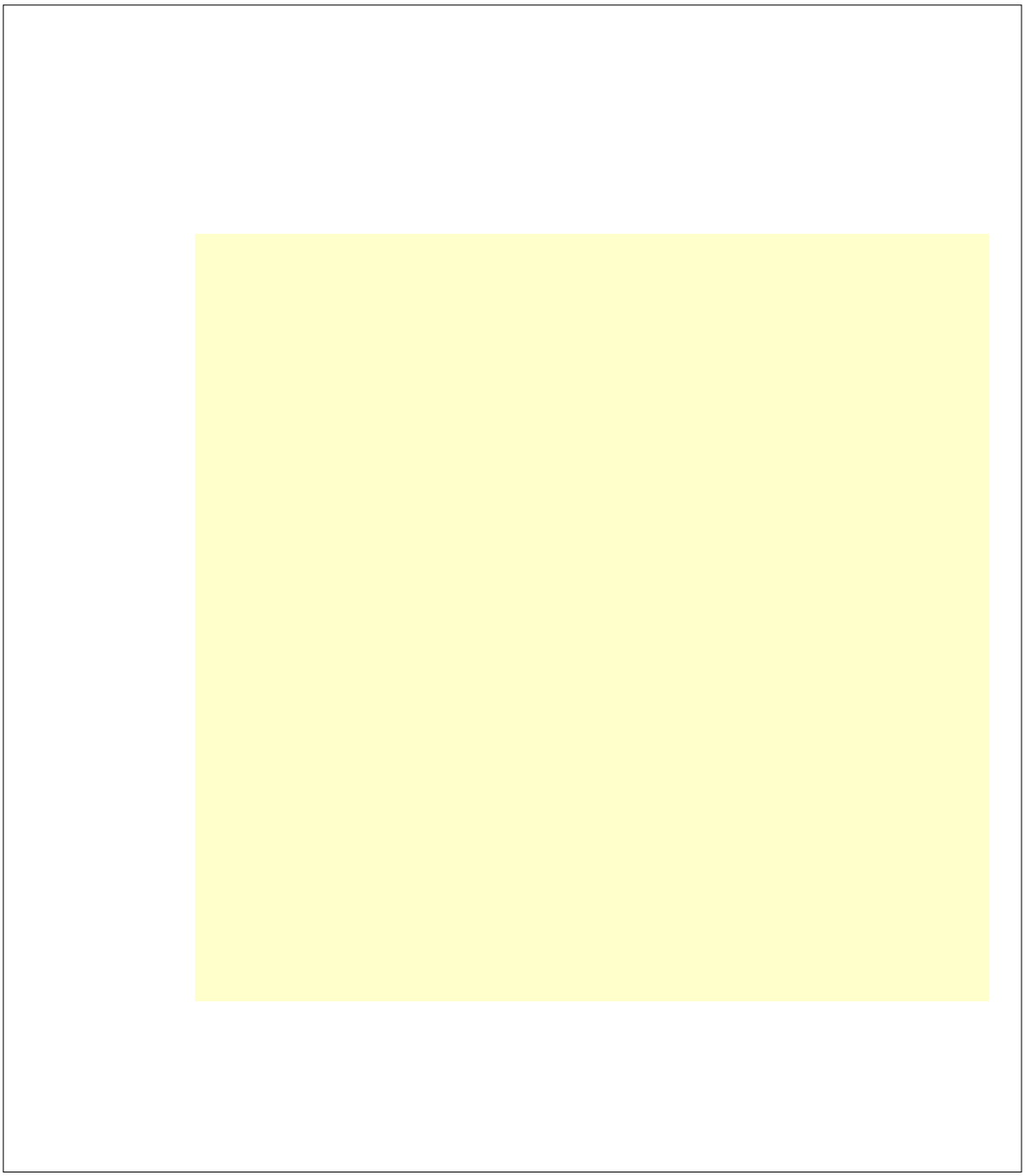
(In principle, it is possible to construct a Schrödinger equation, , $\Psi = E\Psi$, to describe the electronic structure of a molecule.

; In practice, seeking exact solutions to the Schrödinger equation for molecules is an insurmountable mathematical problem.

L Two principal approaches have been taken to construct approximate wave functions for molecules, starting with the atomic orbitals of the atoms comprising the molecules.

1. Valence Bond (VB) theory - developed by Linus Pauling and co-workers, essentially puts the Lewis notion of

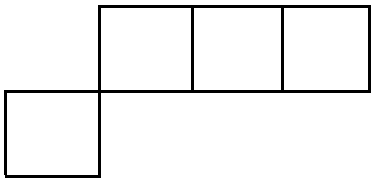
Valence Bond (VB) Theory

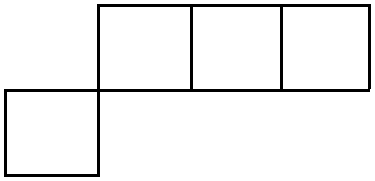


Heteronuclear Diatomic Molecules

- In heteronuclear diatomic molecules, the overlap may involve two different types of orbitals.

Hybrid Orbital Formation in CH





s *p* *sp* orbitals (2)