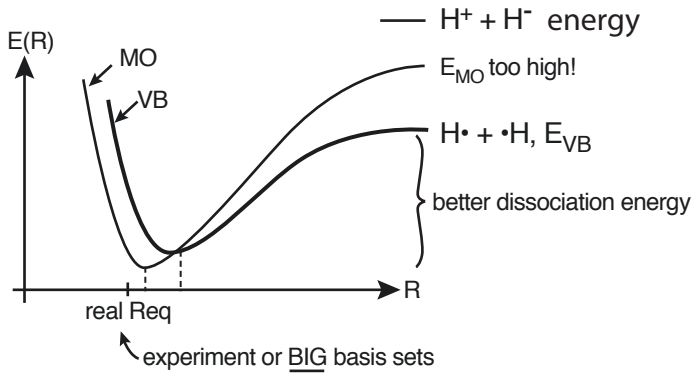
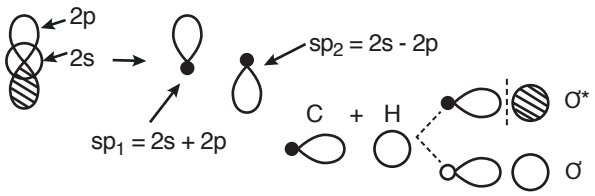
Valence bond vs. MO basis function:

Leave out "ionic terms" in the MO wavefunction that put both electrons on the same atom, to obtain more realistic bond dissociation into two neutral fragments, H• + •H

Potential energy surfaces E(R) (or V(R)) for the MO and VB wavefunctions:



Another example of atom-localized basis sets: sp hybrid orbitals



An extreme example of localization: limit of ∞ electron mass and Lewis dots: