Slater Type Orbitals

A bond is a small perturbation on an atom.[1]

Use simpler wavefunctions that have appropriate large r behavior. Bond formation involves overlap of atomic orbitals at large r.

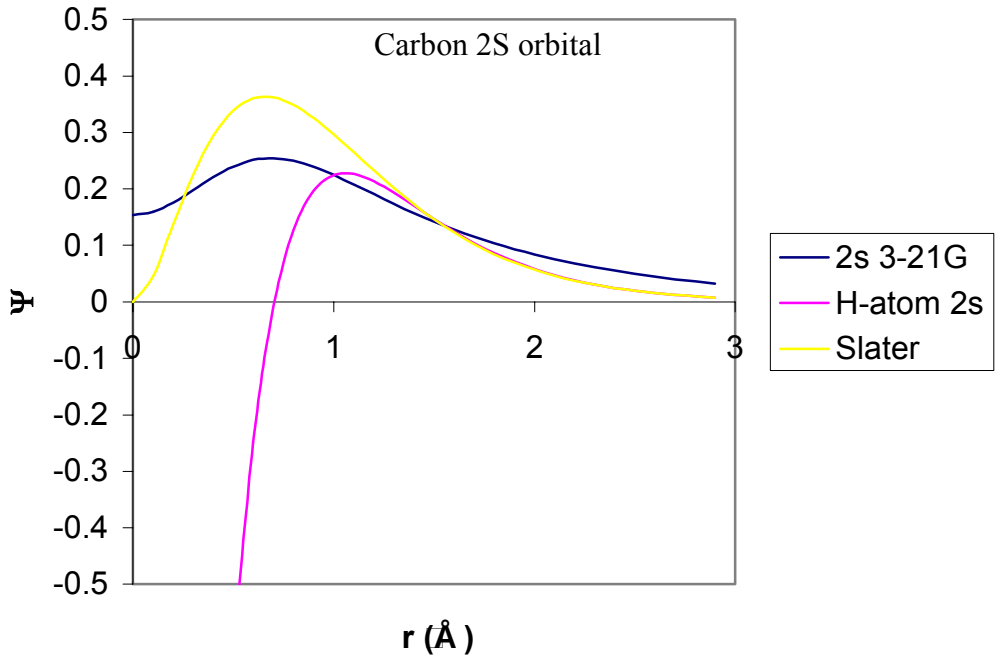
Slater Type Orbitals, STO

$$\Psi_{nlm}(r) = N\, Y_{lm}(\theta,\phi)\, r^{(n-1)}\, e^{-Z_{eff}\, r/\, n\, a_o}$$

For He $Z_{eff} = 1.6875$

Slater Orbital Parameters Z_{eff}. (ref. 2)

	Li	Be	B	C	N	O	F
Z	3	4	5	6	7	8	9
1s	2.6906	3.6843	4.6795	5.6727	6.6651	7.6579	8.6501
2s	1.2792	1.9120	2.5762	3.2166	3.8474	4.4916	5.1276
2p			2.4214	3.1358	3.8340	4.4532	5.1000



1. I don't know who said this first. I heard it from Warren Hehre.
2. John S. Winn, *Physical Chemistry*, Harper Collins, New York, NY, 1995, p. 472