

CHEM302
Introduction to Computational
Chemistry

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Spring 2010

Slater-type orbitals (basis functions)

$$\psi_{\text{H}1s} = \frac{1}{\sqrt{\pi}} e^{-r}$$

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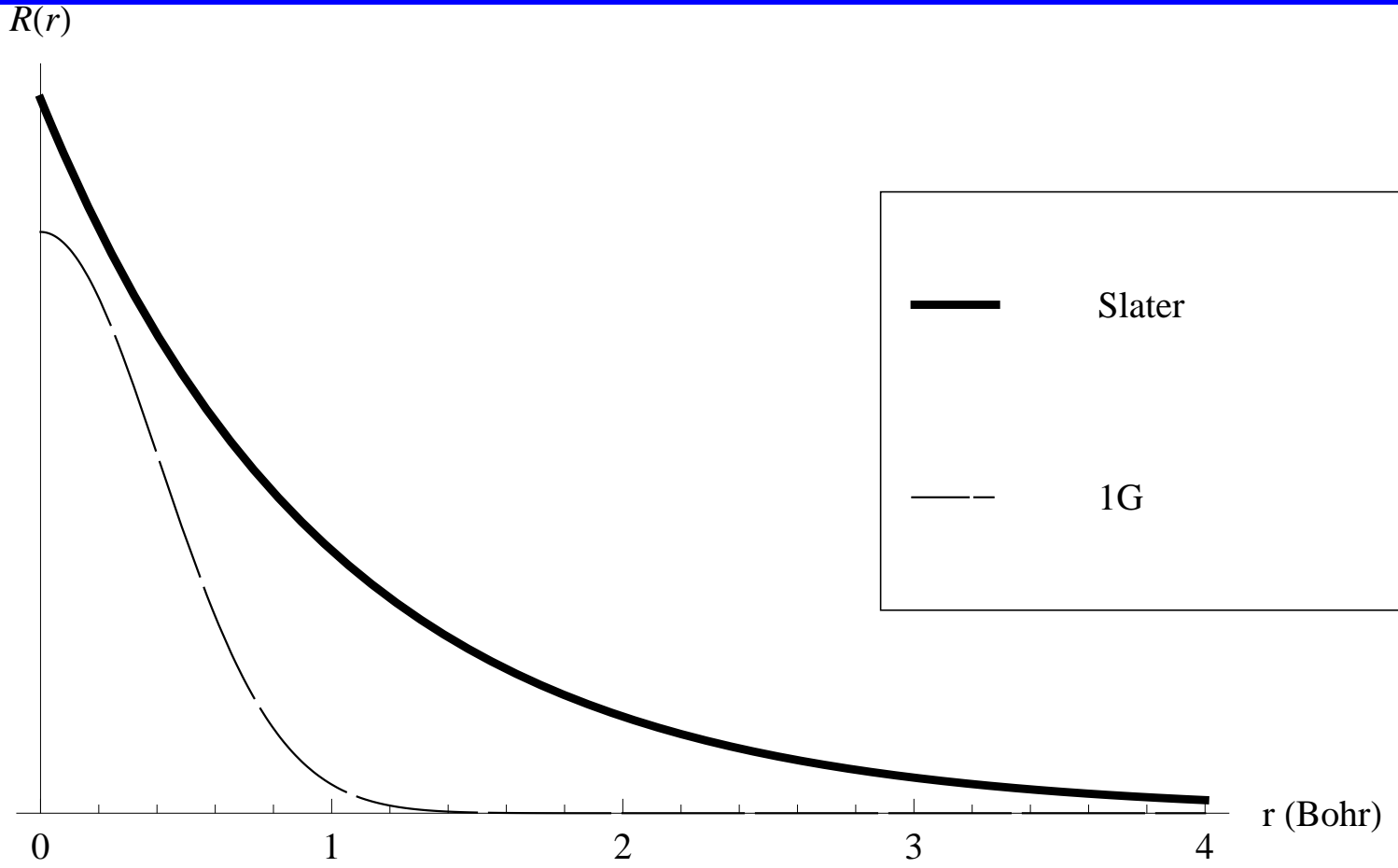
$$\psi_{\text{H}1s} = \frac{1}{\sqrt{\pi}} e^{-r}$$
$$\phi_{\text{STO}1s} = 2\zeta^{3/2} e^{-\zeta r}$$

Gaussian-type orbitals (basis functions)

$$\phi_{\text{GTO}1s} = \left(\frac{2}{\pi} \right)^{3/4} \alpha^{3/4} e^{-\alpha r^2}$$

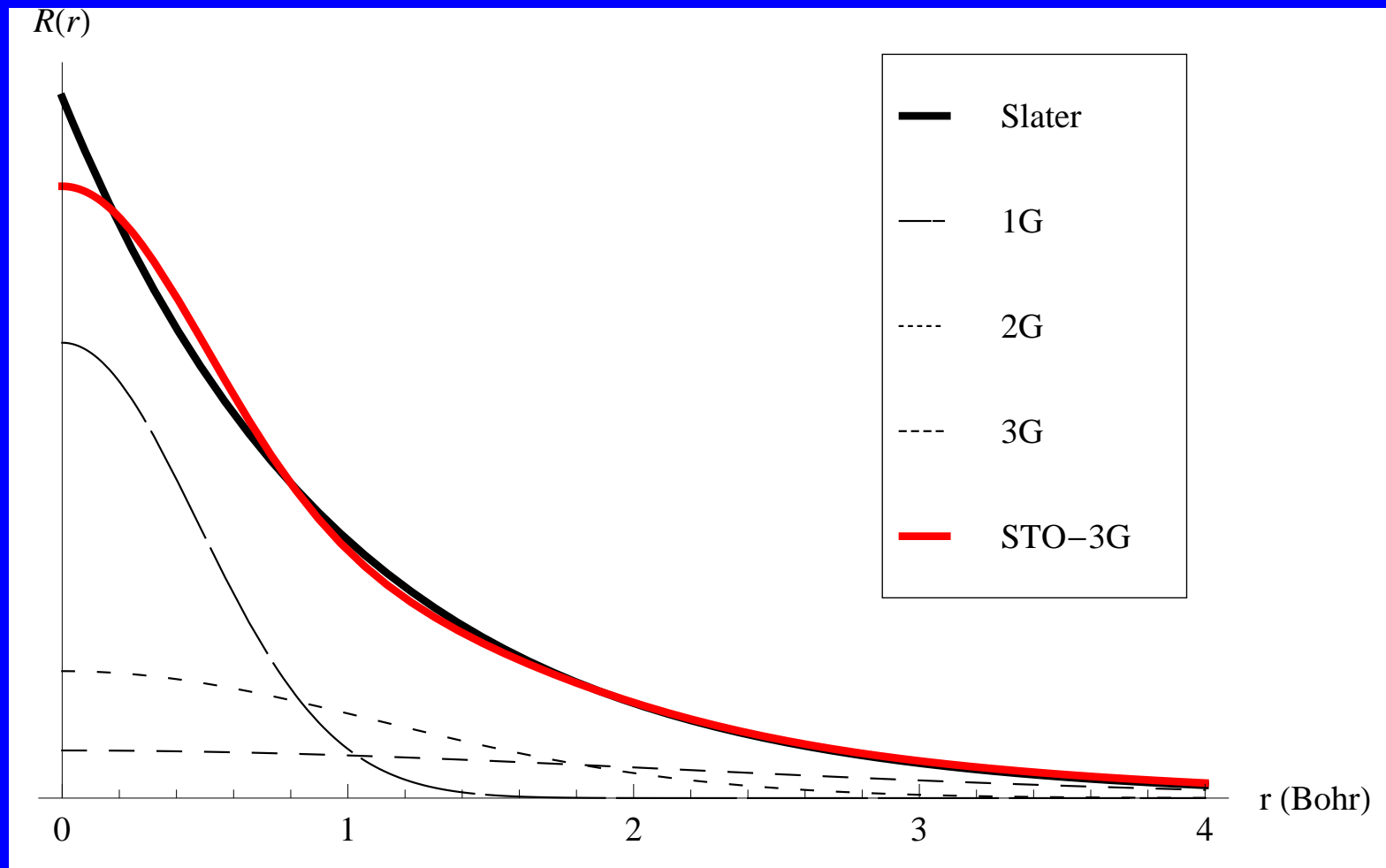
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Gaussian-type orbitals (basis functions)

$$\varphi_{\text{STO-3G}1s} = c_1\phi_1 + c_2\phi_2 + c_3\phi_3$$



Gaussian-type orbitals (basis functions)

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- decontraction

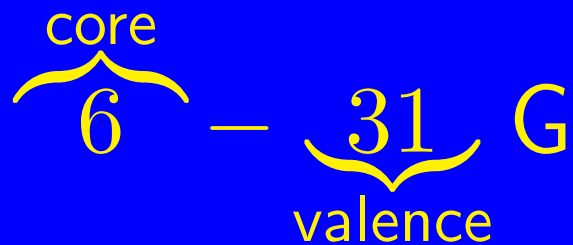
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- single- ζ , double- ζ , triple- ζ , etc.

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- split-valence

Pople split-valence basis sets



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3-21G, 6-311G

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15: 3 for the 1s, 2 for 1 2s, 1 for the other, 2 for each of a set of 3 2p's, 1 for each in the second set of 2p's

Polarization functions

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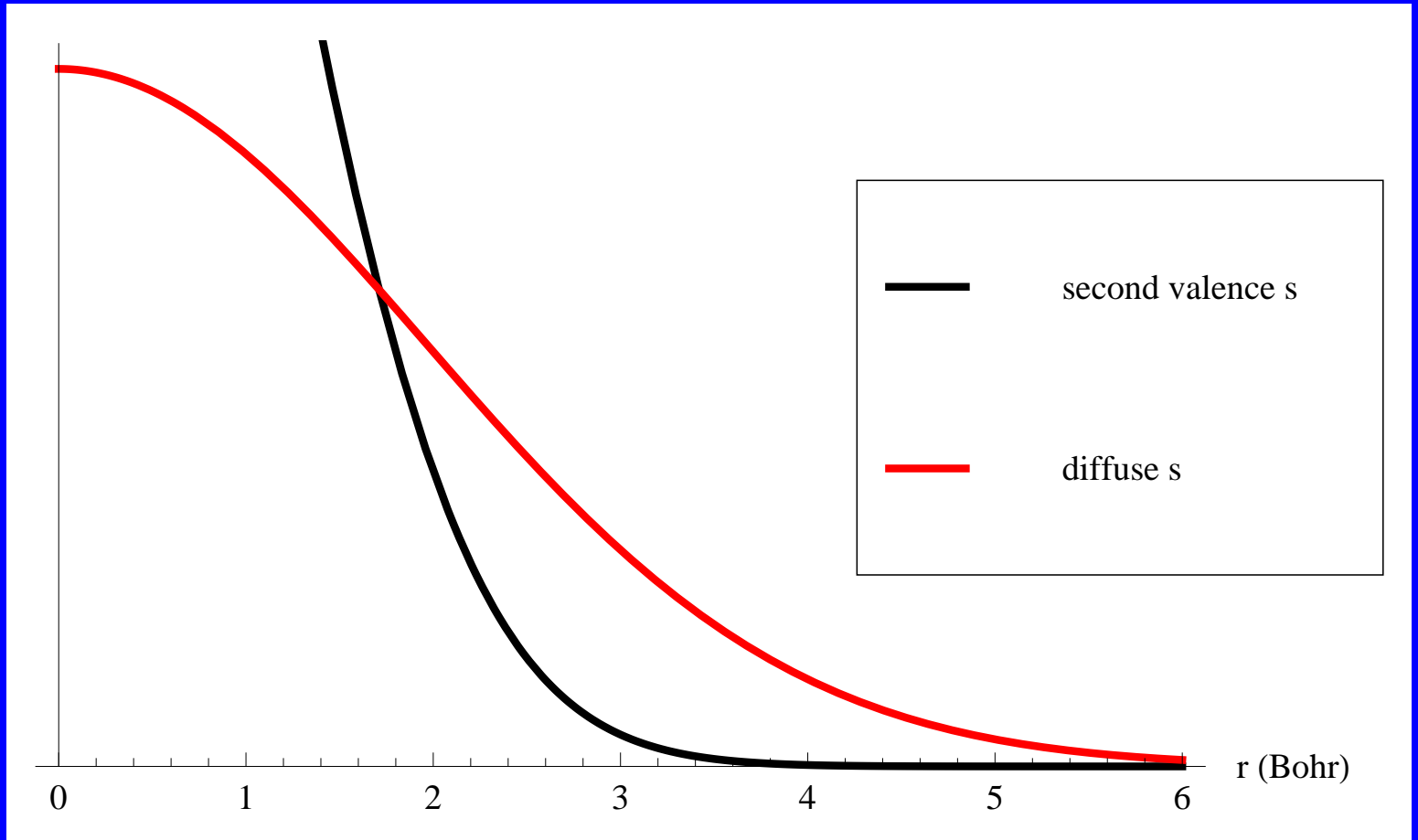
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6-311G(d), 6-311G(d,p)

Balance: 6-311G(2df), 6-311G(2df,2pd)

Diffuse functions



6-31+G

Favorite Pople type basis sets

- 6-31G(d)
- 6-31+G(d,p) (DIDZ)
- 6-31++G(d,p) (QCRNA)
- 6-311+G(2df,2p) (MSG3S)
- 6-311++G(2df,2p) (MSG3)

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Diffuse functions (one of each type) can be added.

Effective-core potentials (ECP)

Examples:

LanL2MB: STO-3G on 1st and 2nd row, Los Alamos ECP plus a minimal basis on remaining

LanL2DZ: D95V on 1st and 2nd row, Los Alamos ECP plus a double- ζ basis on remaining