Comparison of VQE methods for ground state energy

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$$H = \sum_{\alpha \in \{\uparrow,\downarrow\}} \sum_{pq} c_{pq} a^{\dagger}_{p,\alpha} a_{q,\alpha} + \frac{1}{2} \sum_{\alpha,\beta \in \{\uparrow,\downarrow\}} \sum_{pqrs} c_{pqrs} a^{\dagger}_{p,\alpha} a^{\dagger}_{q,\beta} a_{r,\beta} a_{s,\alpha}$$

where **α** and **β** denote the electron spin and p, q, r, s are the orbital indices. The coefficients c are integrals over molecular orbitals that are obtained from Hartree–Fock calculations.

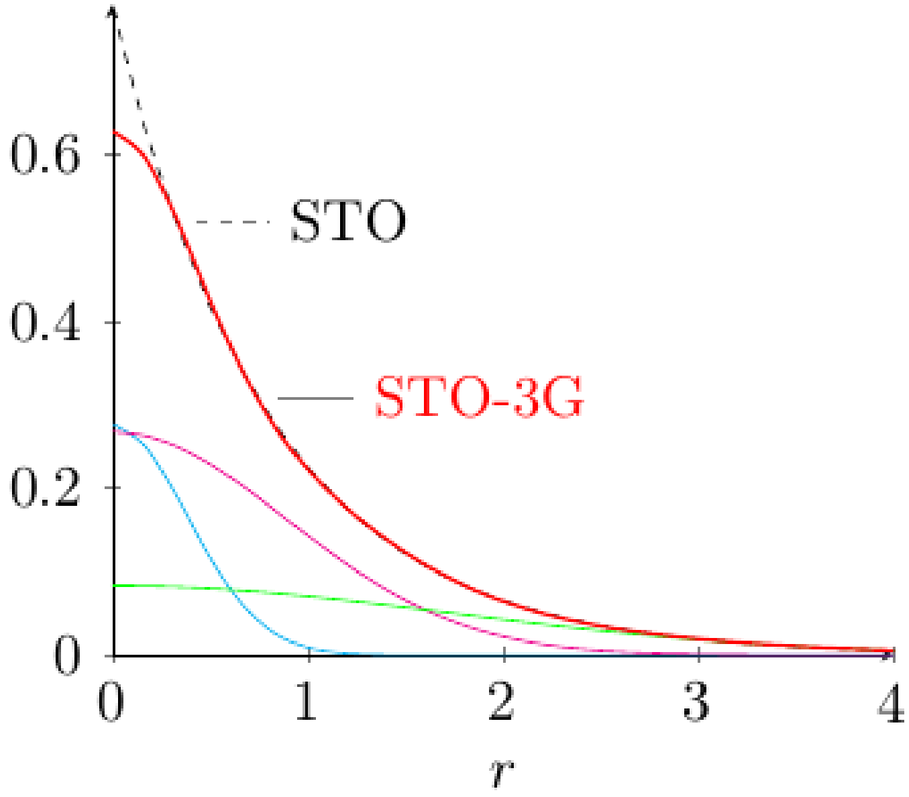
Basis sets
– STO-3G, STO-6G…

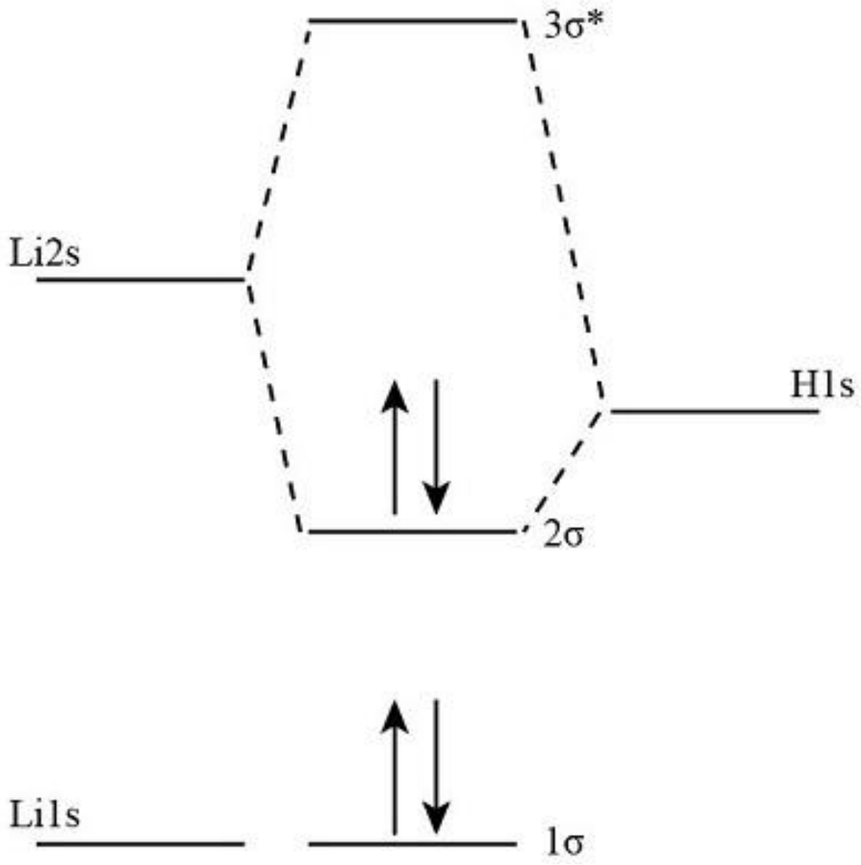
- Slater-type orbital

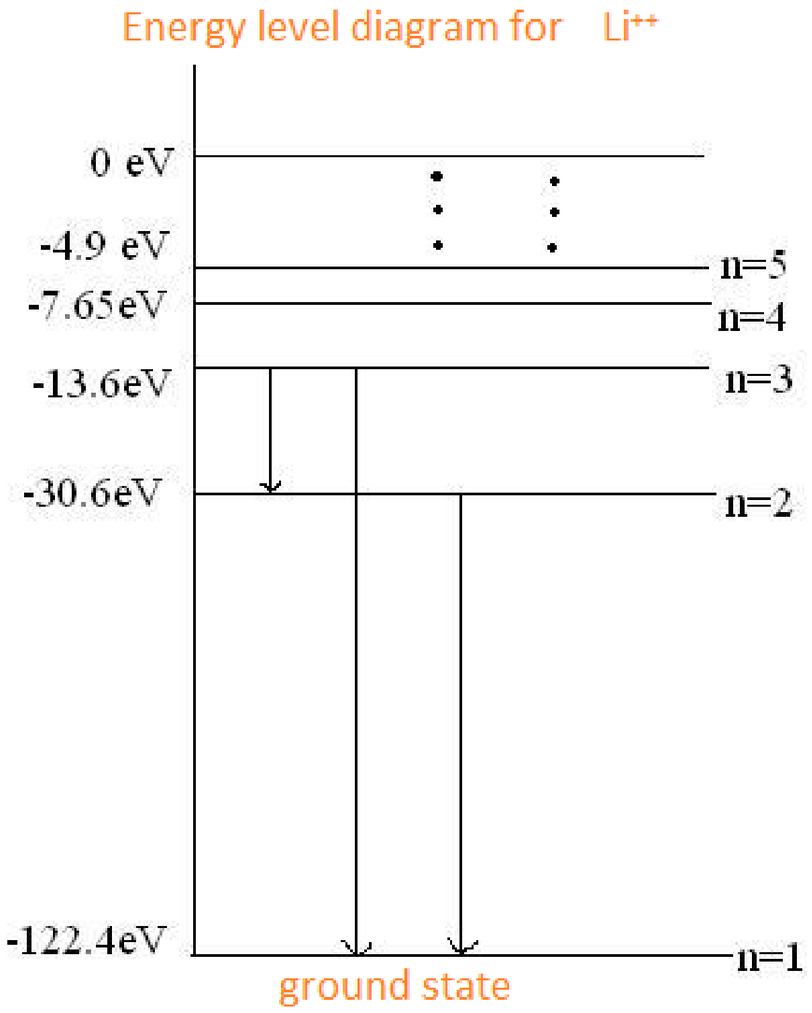
$$R_n^{\mathrm{STO}}(r) \propto (\zeta r)^{n-1} e^{-\zeta r}$$

- Gaussian-type orbital

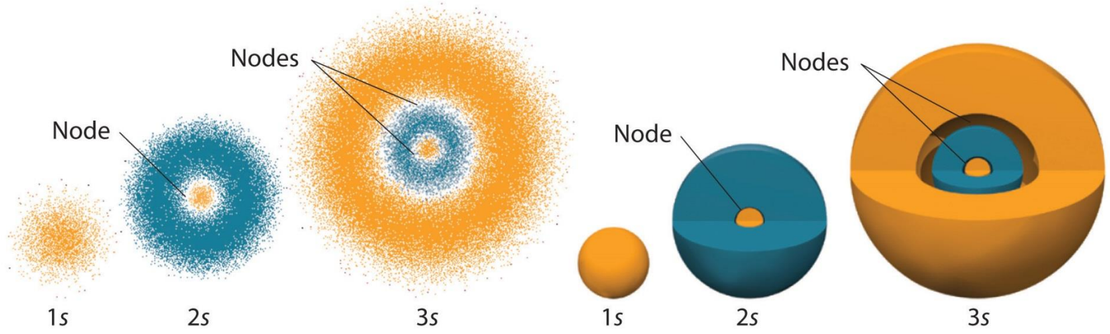
$$R_{nl}^{\mathrm{GTO}}(r) \propto (\sqrt{\alpha_{nl}} r)^{l} e^{-\alpha_{nl} r^2}$$




3σ*
Li2s
H1s
2σ
Li1s
1σ

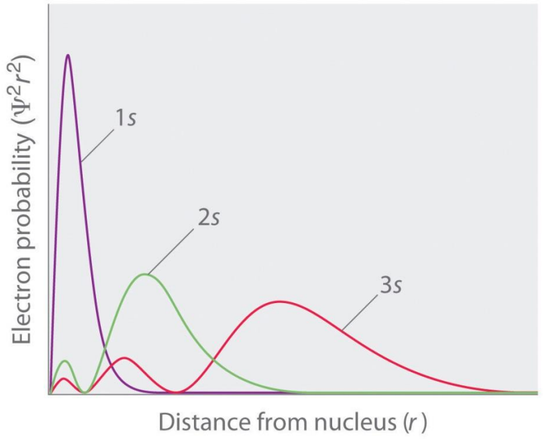

Energy level diagram for Li++
0 eV
-4.9 eV
-7.65eV
-13.6eV
-30.6eV
-122.4eV
n=5
n=4
n=3
n=2
n=1
ground state

Orbital probability density function



(a) Electron probability

(b) Contour probability



(c) Radial probability

THANK YOU