

Shielding in Li $1s^22s$ and Li $1s^22p$

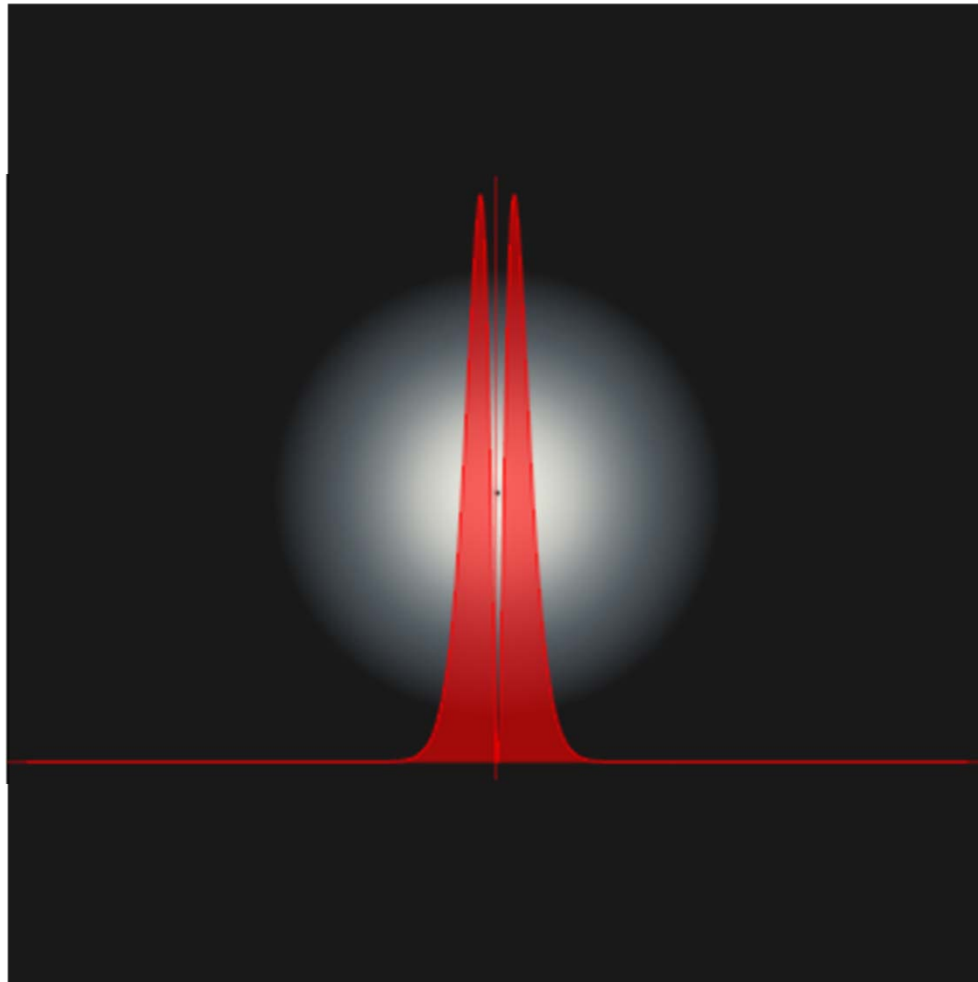
CH101 Fall 2012
Boston University

The Li atom electron configuration 1s²2s is more stable than 1s²2p.

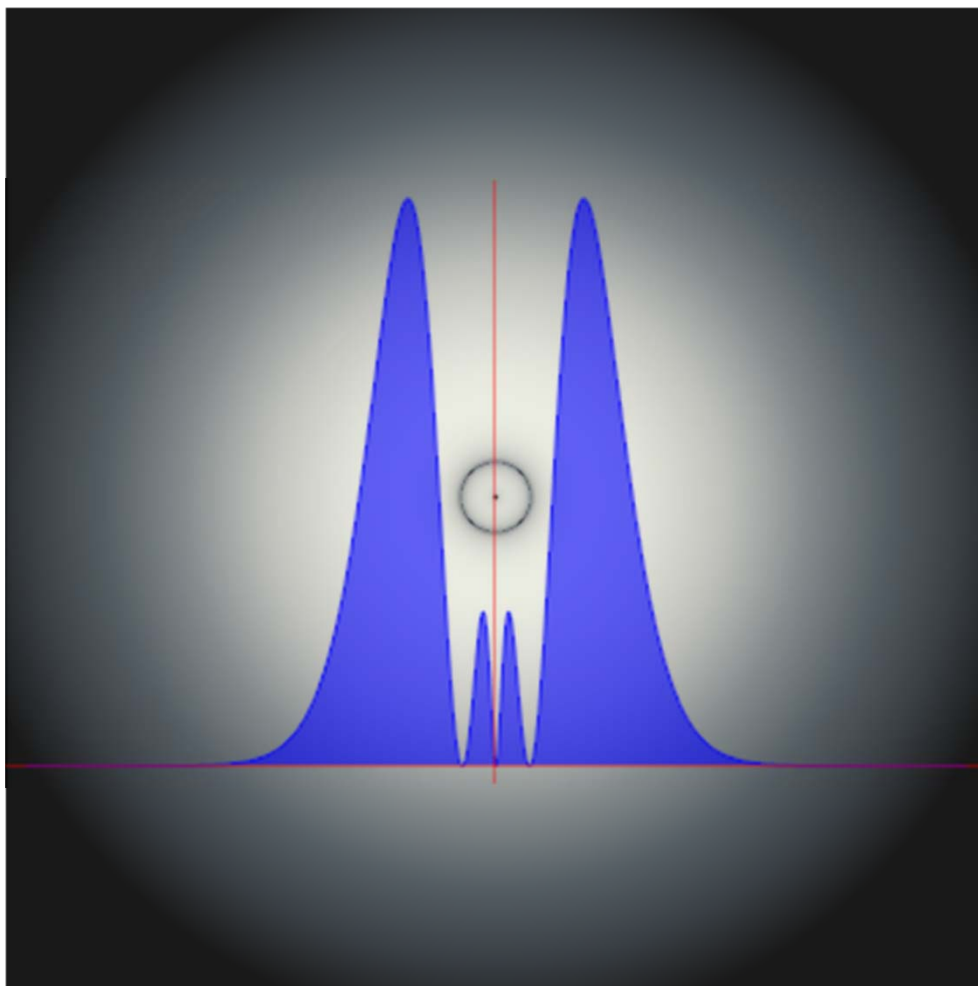
The reason is, the 2s electron feels a greater nuclear charge, Z_{eff} , than does the 2p electron.

The following illustrations show qualitatively why this is so.

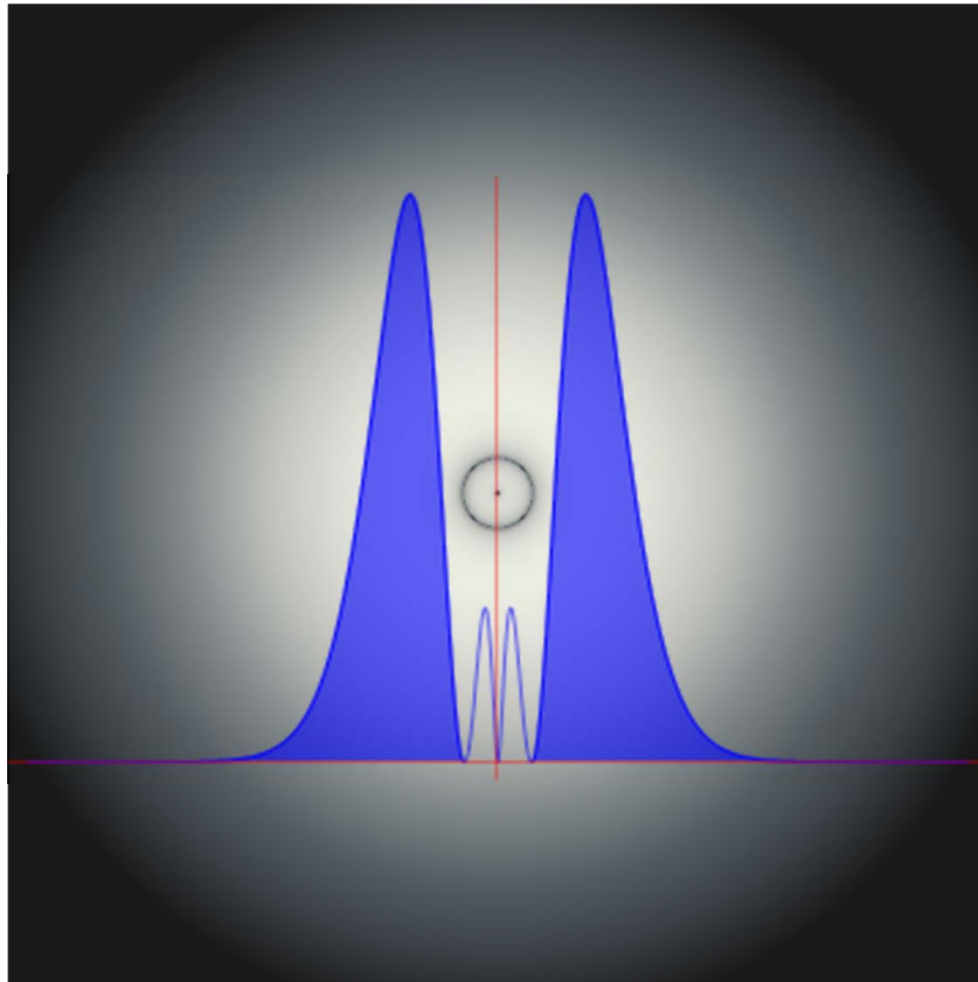
1s² portion of Li electron cloud



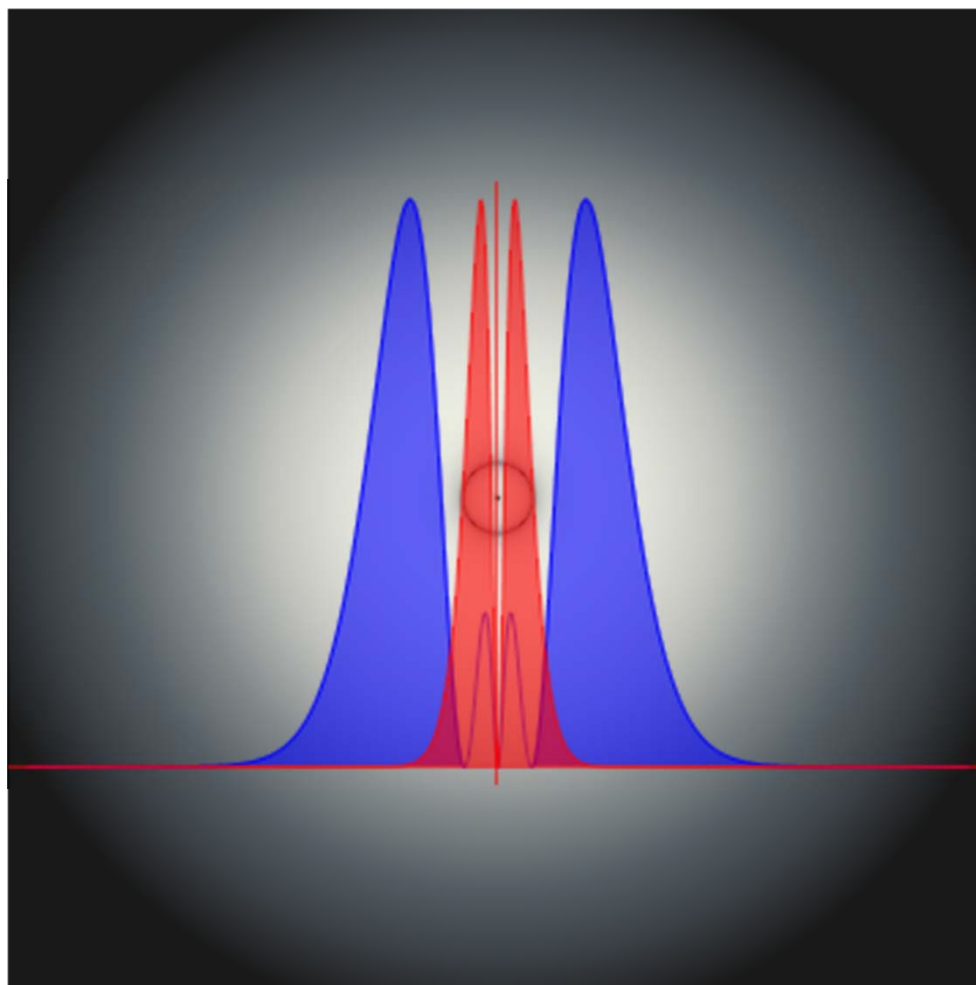
2s portion of Li 1s²2s electron cloud



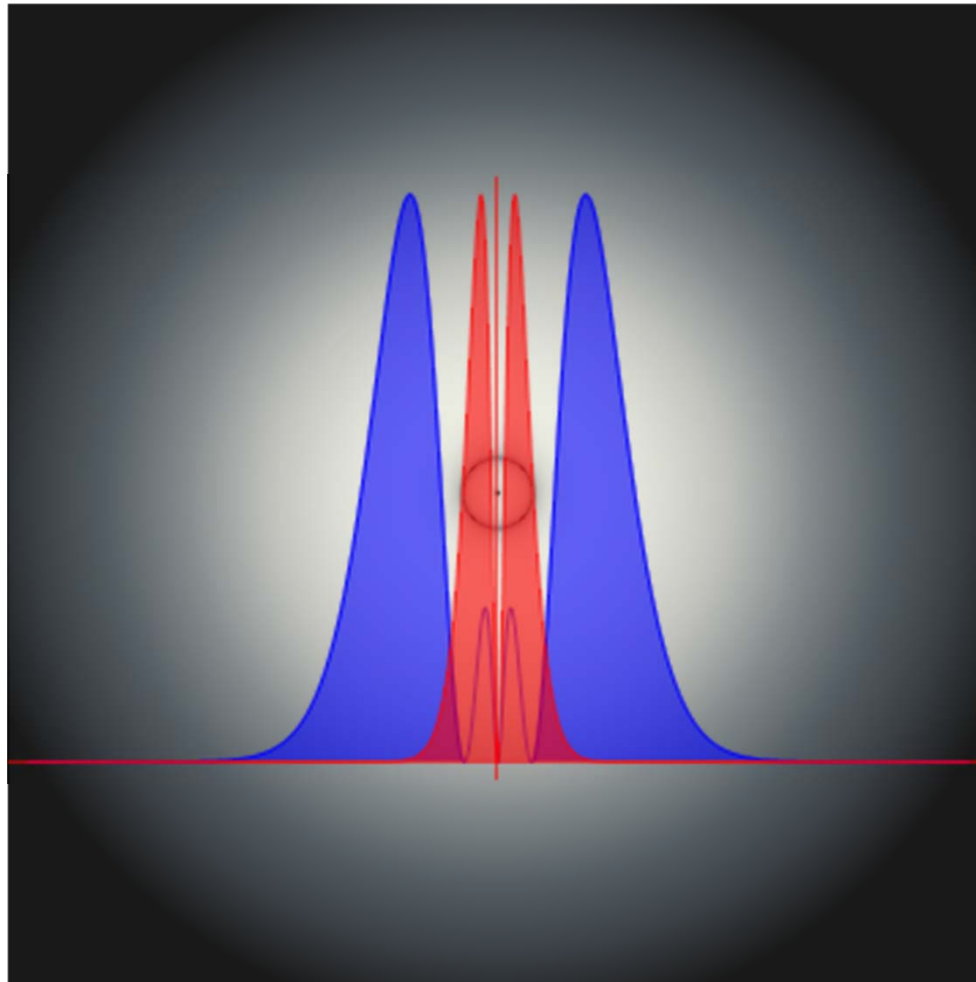
2s outer loop of Li 1s²2s electron cloud



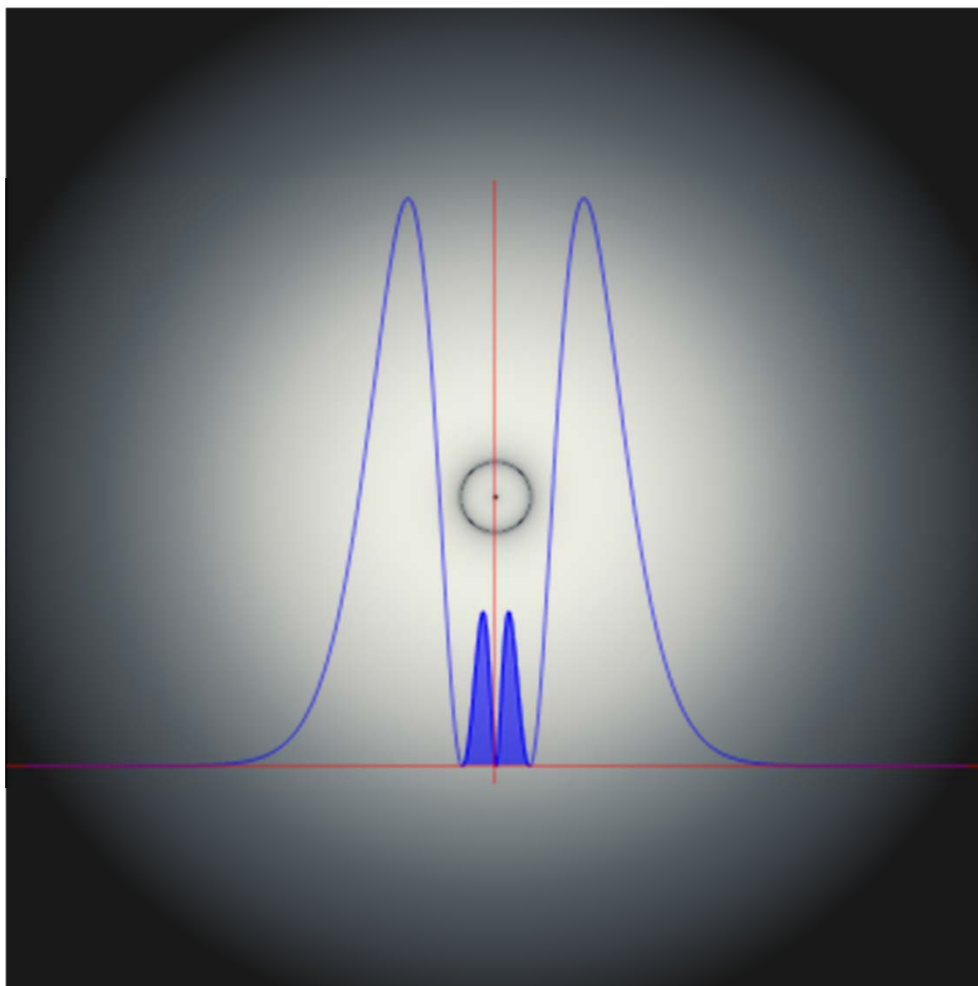
2s outer loop is shielded by 1s² cloud



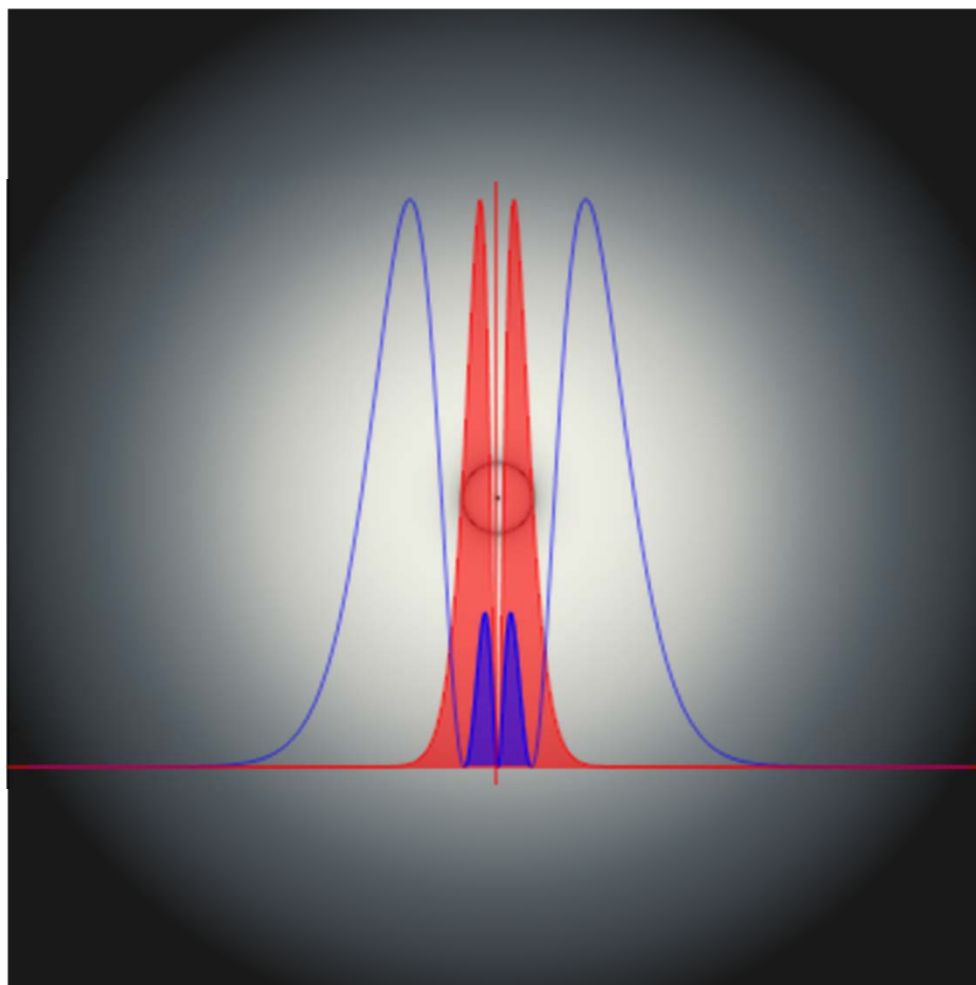
For ~90% of 2s, $Z_{\text{eff,outer}} \approx 0.90 \times (3 - 2) = 0.9$



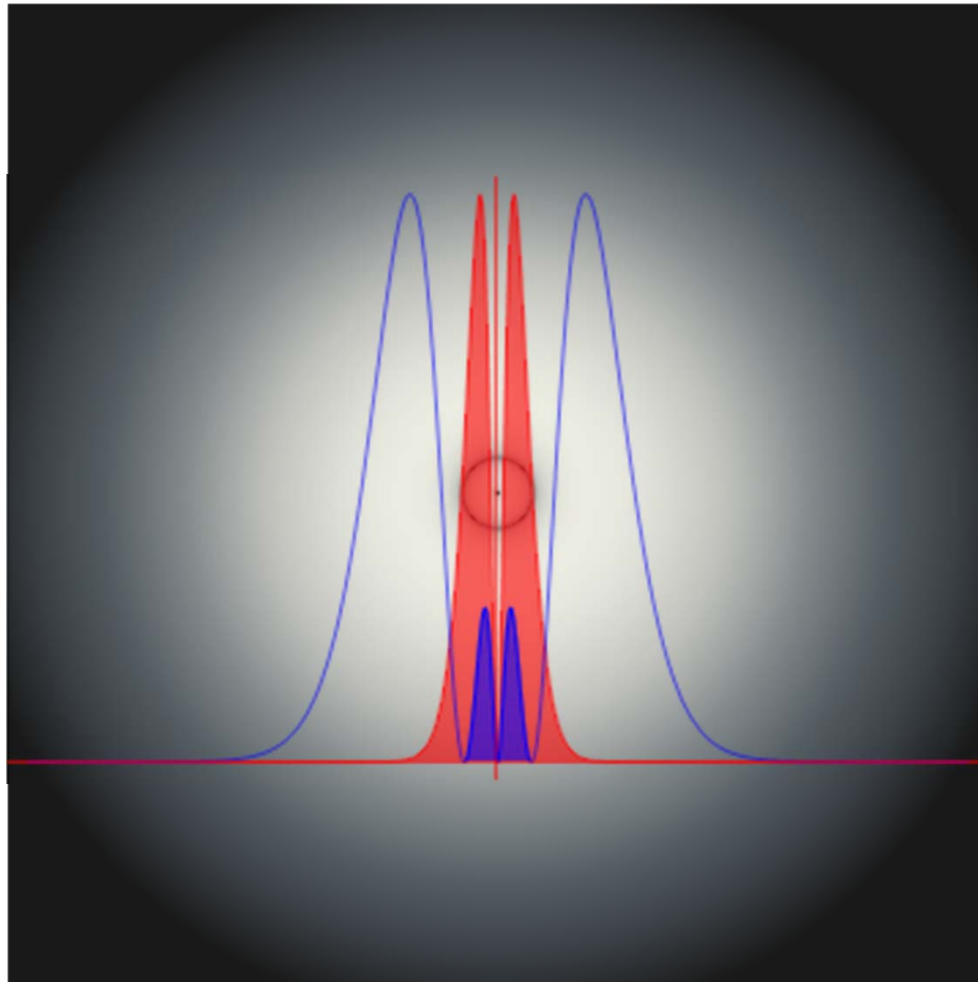
2s inner loop of Li 1s²2s electron cloud



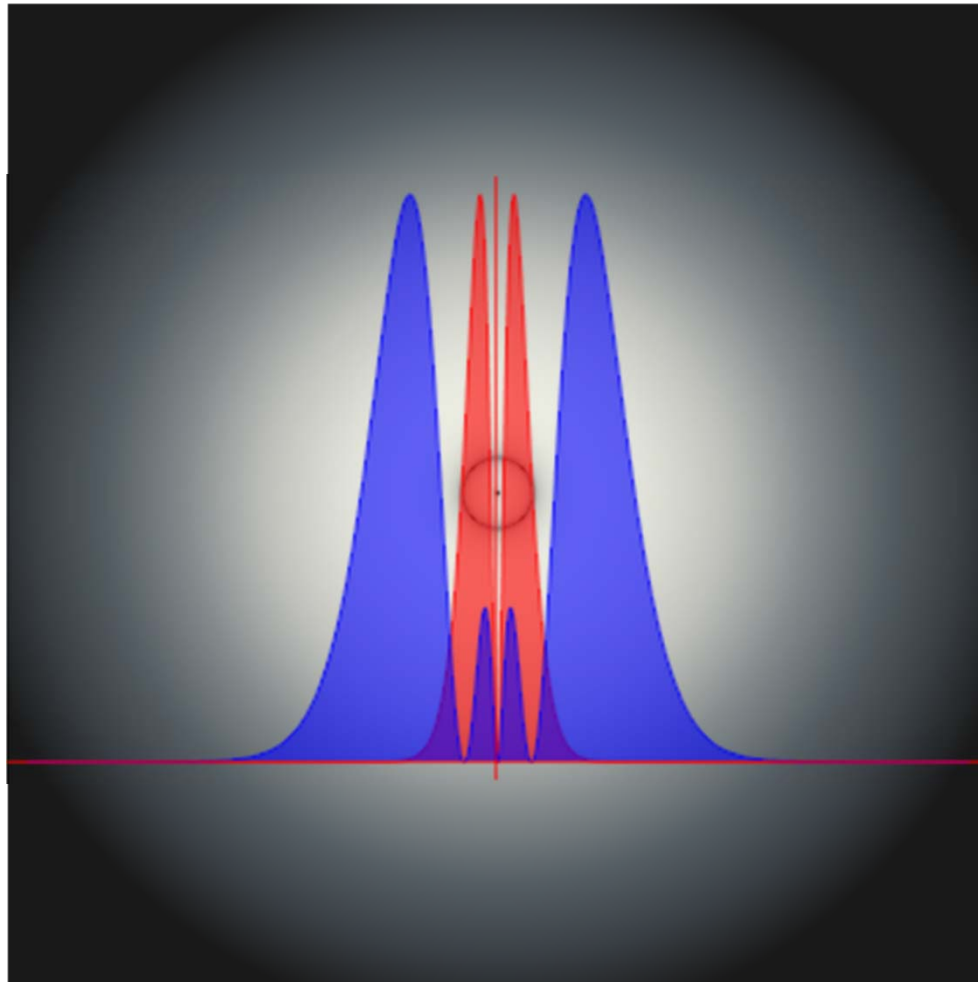
2s inner loop is **not shielded** by 1s² cloud



For ~10% of 2s, $Z_{\text{eff,inner}} \approx 0.10 \times 3 = 0.3$



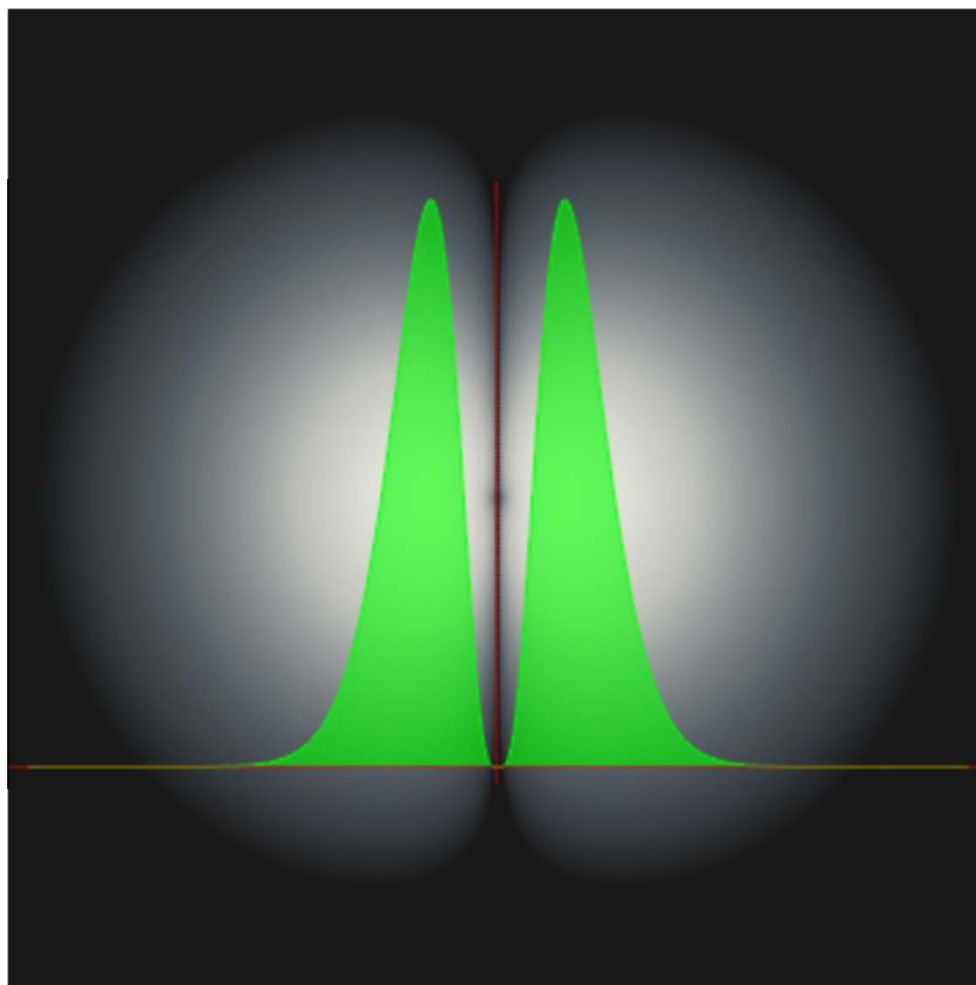
$$Z_{\text{eff},2s} = Z_{\text{eff},\text{outer}} + Z_{\text{eff},\text{inner}} = 0.9 + 0.3 = 1.2$$



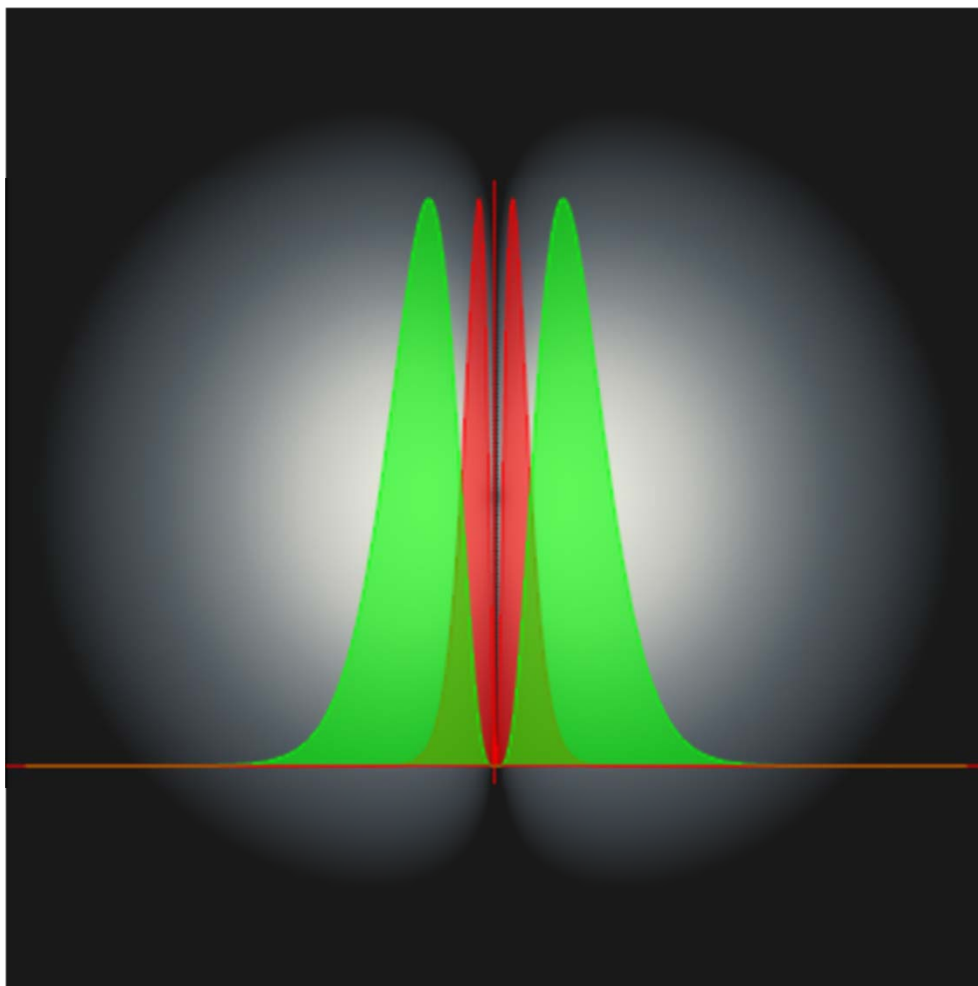
Li 1s²2s valence electron energy

$$\begin{aligned} E_{2s} &= -13.6 \text{ eV } Z_{\text{eff},2s}^2/4 \\ &= -13.6 \text{ eV } \times 1.2^2/4 = -4.90 \text{ eV} \end{aligned}$$

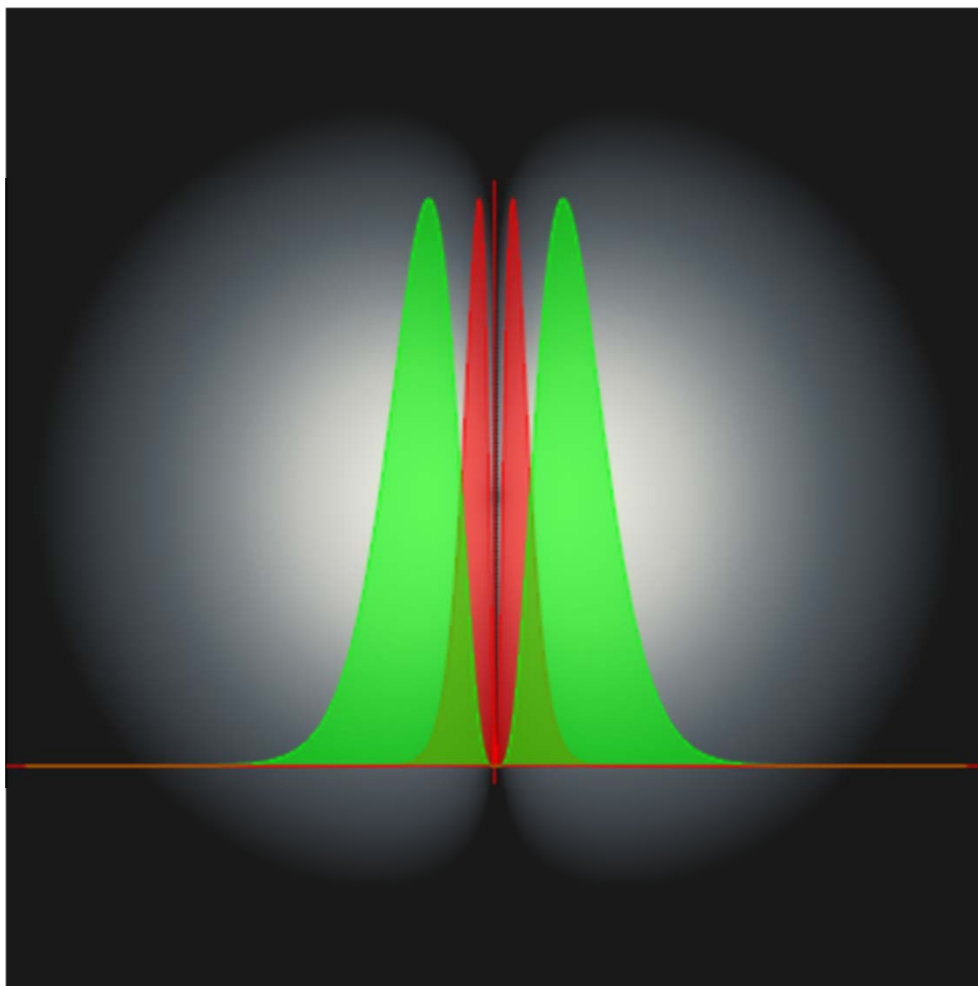
2p portion of Li 1s²2p electron cloud



2p is shielded by 1s² cloud



For ~100% of 2p, $Z_{\text{eff},2p} \approx 1 \times (3 - 2) = 1$



Li 1s²2p valence electron energy

$$\begin{aligned} E_{2p} &= -13.6 \text{ eV } Z_{\text{eff},2p}^2/4 \\ &= -13.6 \text{ eV } \times 1^2/4 = -3.40 \text{ eV} \end{aligned}$$

Li 1s²2s more stable than Li 1s²2p

$$\begin{aligned} E_{2s} &= -13.6 \text{ eV } Z_{\text{eff},2s}^2/4 \\ &= -13.6 \text{ eV } \times 1.2^2/4 = -4.90 \text{ eV} \end{aligned}$$

$$\begin{aligned} E_{2p} &= -13.6 \text{ eV } Z_{\text{eff},2p}^2/4 \\ &= -13.6 \text{ eV } \times 1^2/4 = -3.40 \text{ eV} \end{aligned}$$