Shielding in Li $1s^2 2s$ and Li $1s^2 2p$

CH101 Fall 2012

Boston University

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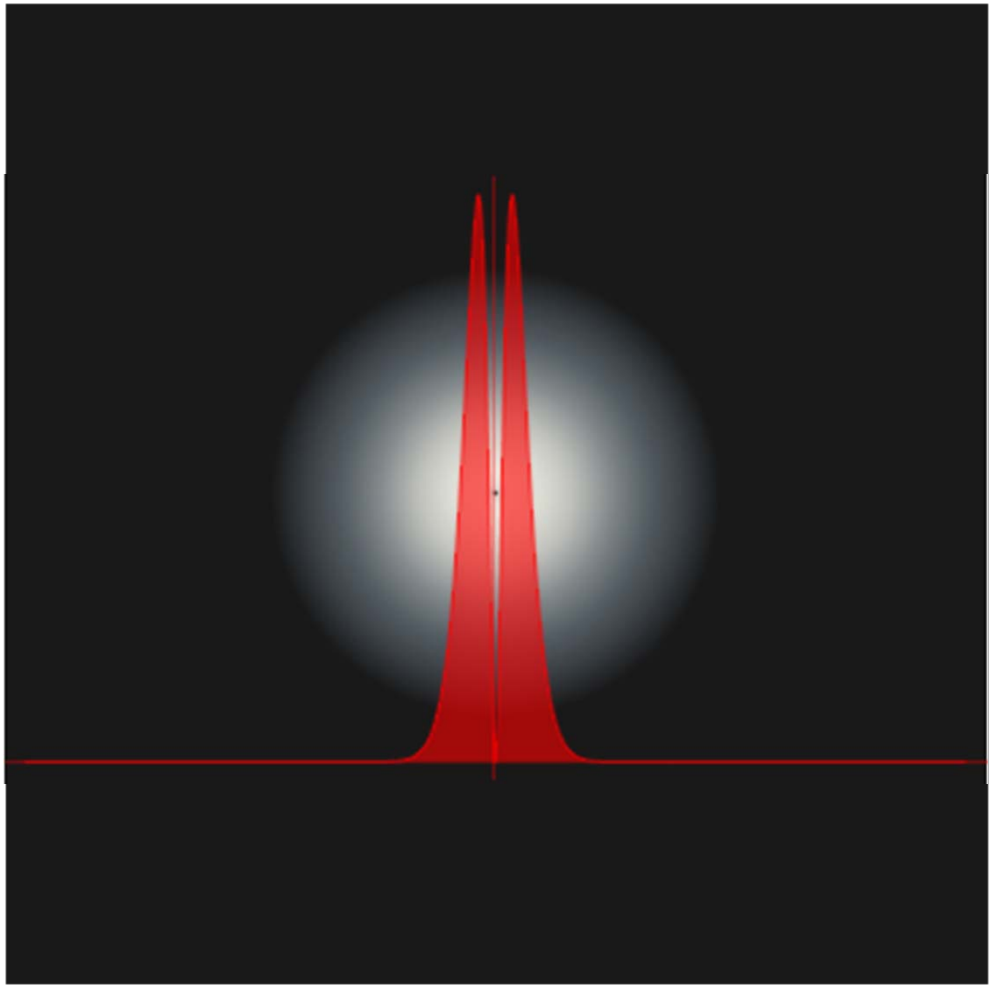
The Li atom electron configuration $1s^2 2s$ is more stable than $1s^2 2p$.

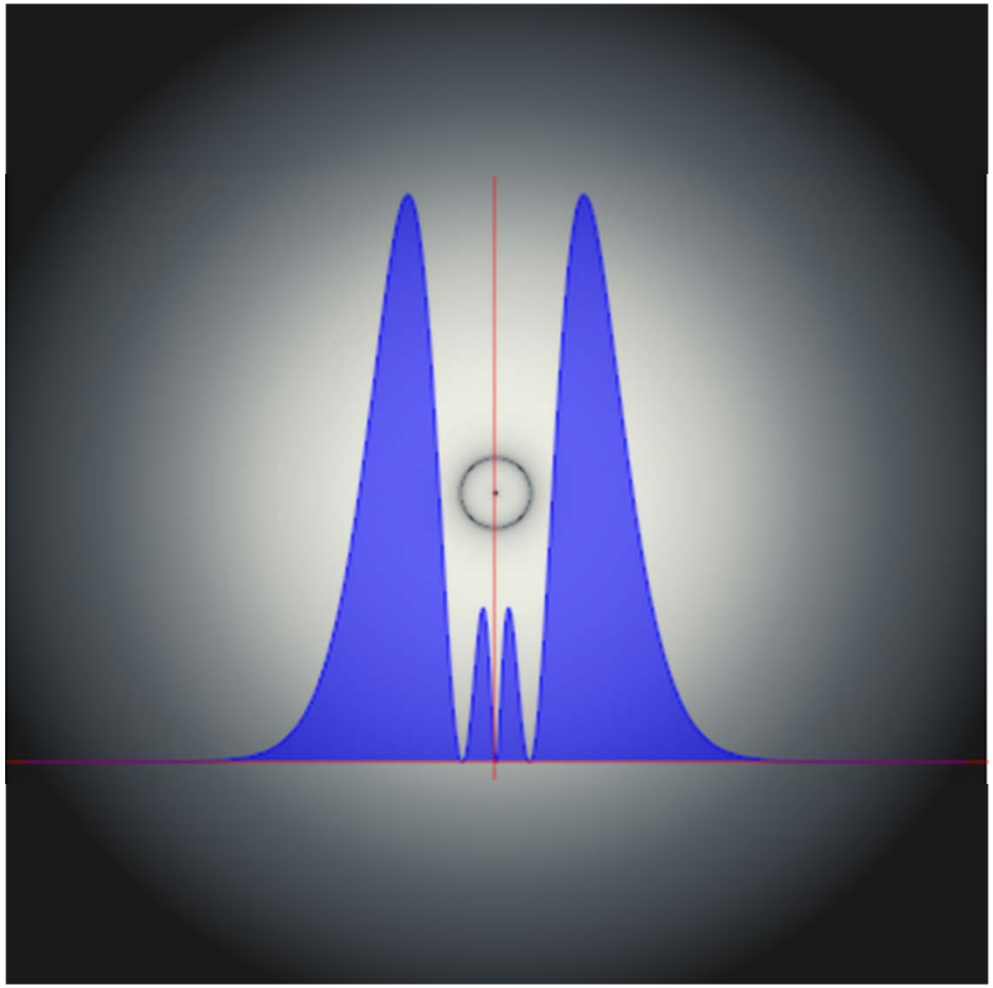
The reason is, the 2s electron feels a greater nuclear charge, Z_{eff}, than does the 2p electron.

The following illustrations show qualitatively why this is so.

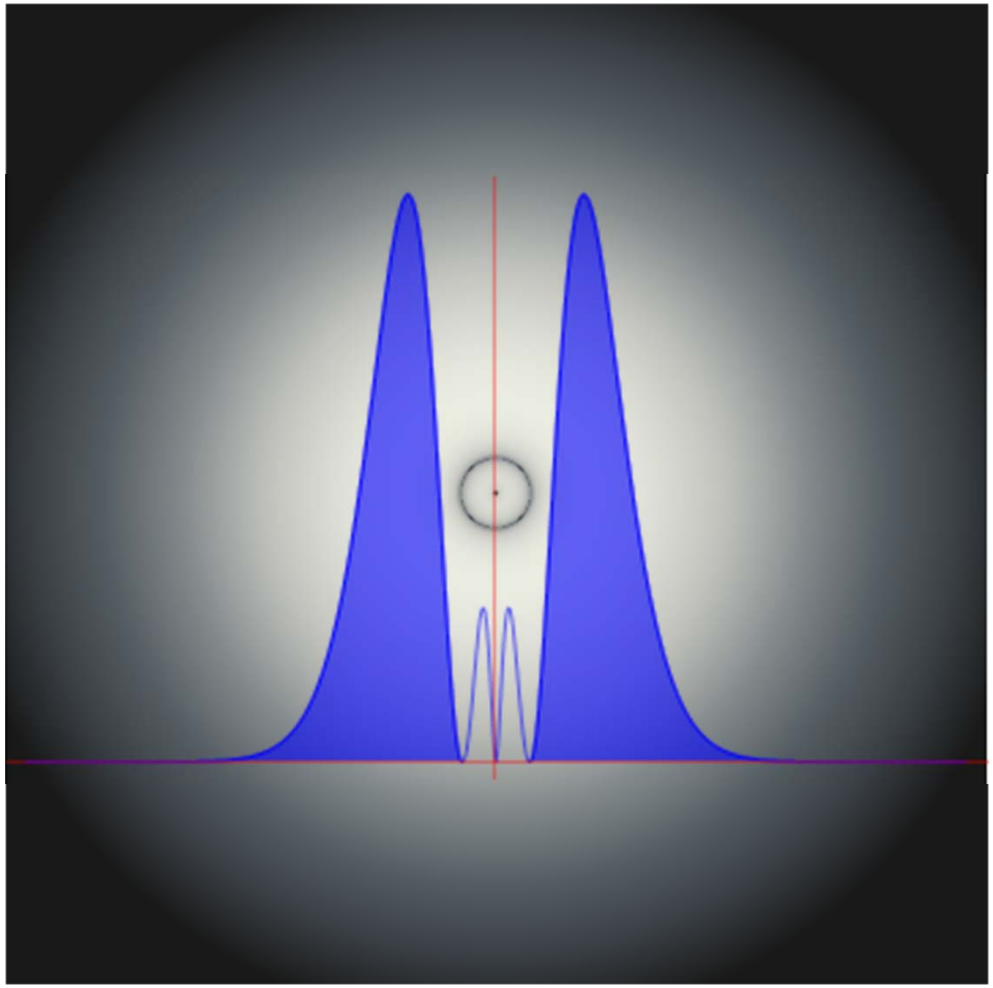
$1s^2$ portion of Li electron cloud



2s portion of Li $1s^2 2s$ electron cloud



2s **outer loop** of Li $1s^2 2s$ electron cloud



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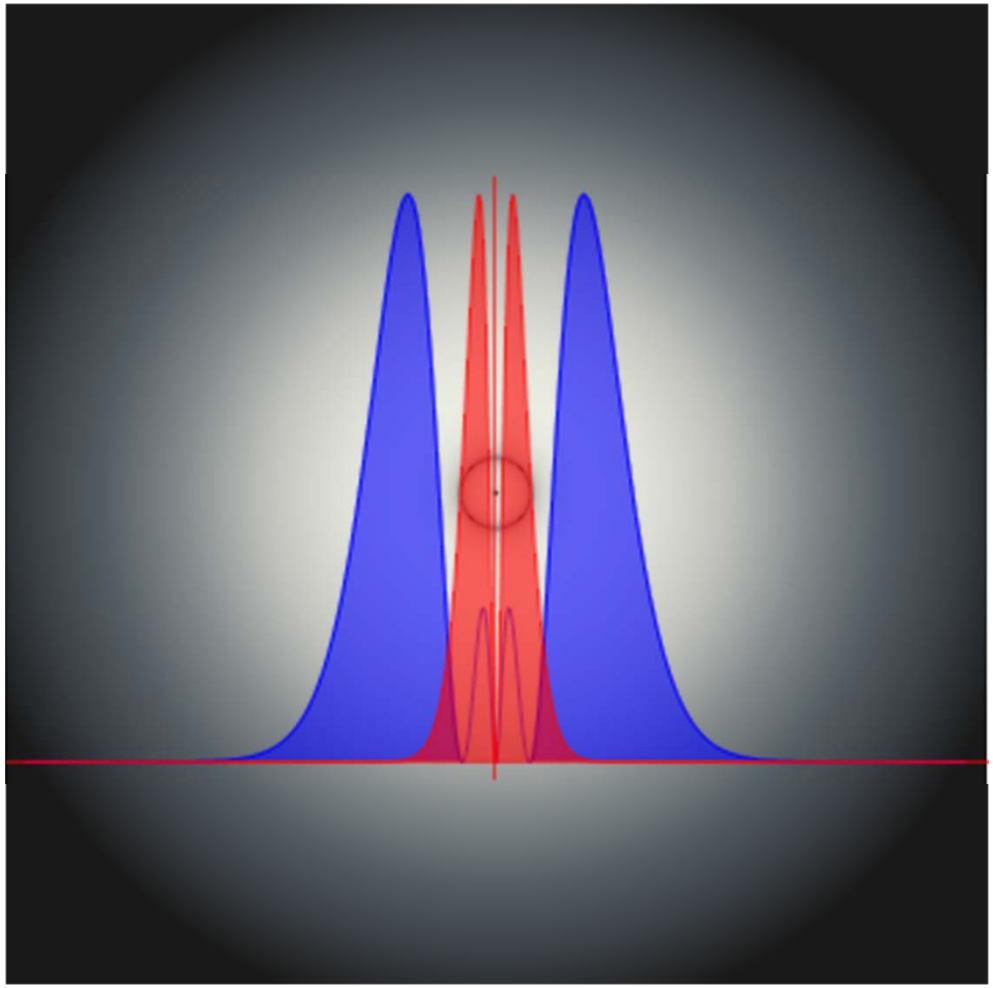
2s **outer loop is shielded** by $1s^2$ cloud



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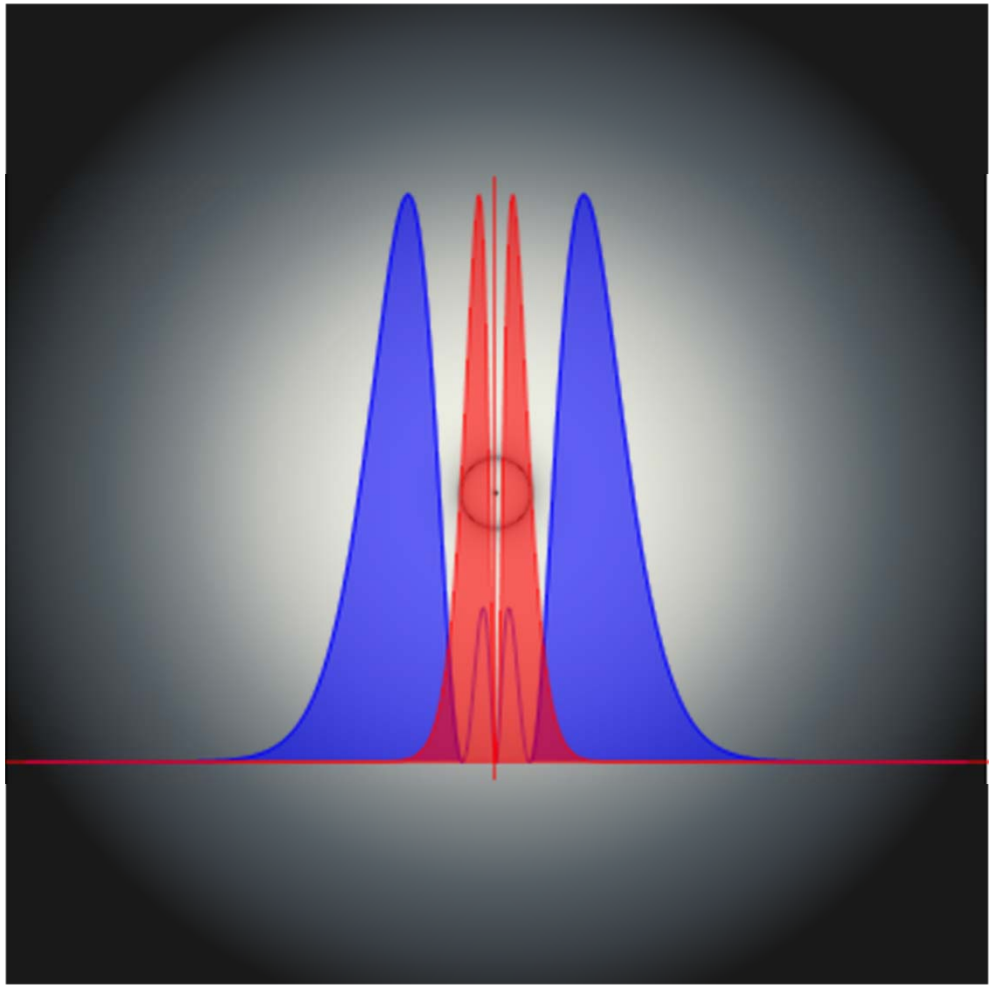
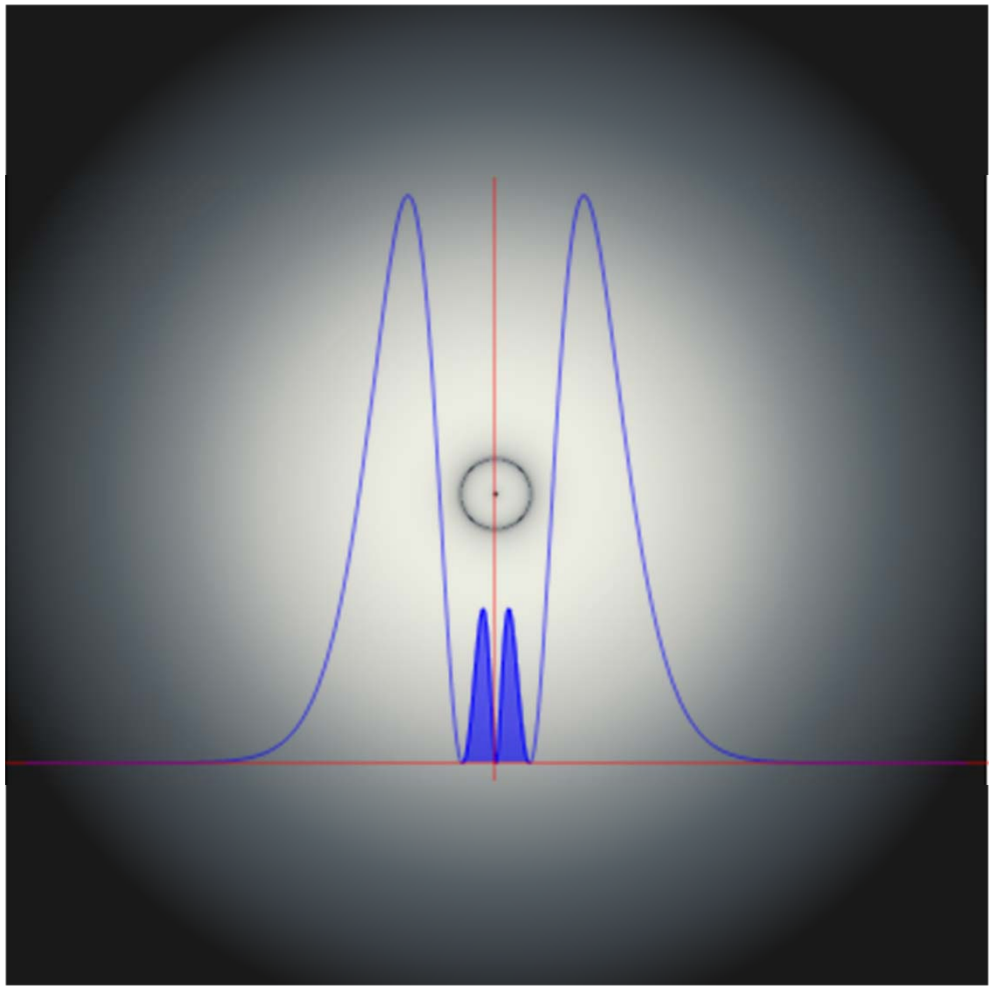
For ~90% of 2s, $Z_{eff,outer} \approx 0.90 \times (3 - \mathbf{2}) = 0.9$



2s **inner loop** of Li $1s^2 2s$ electron cloud



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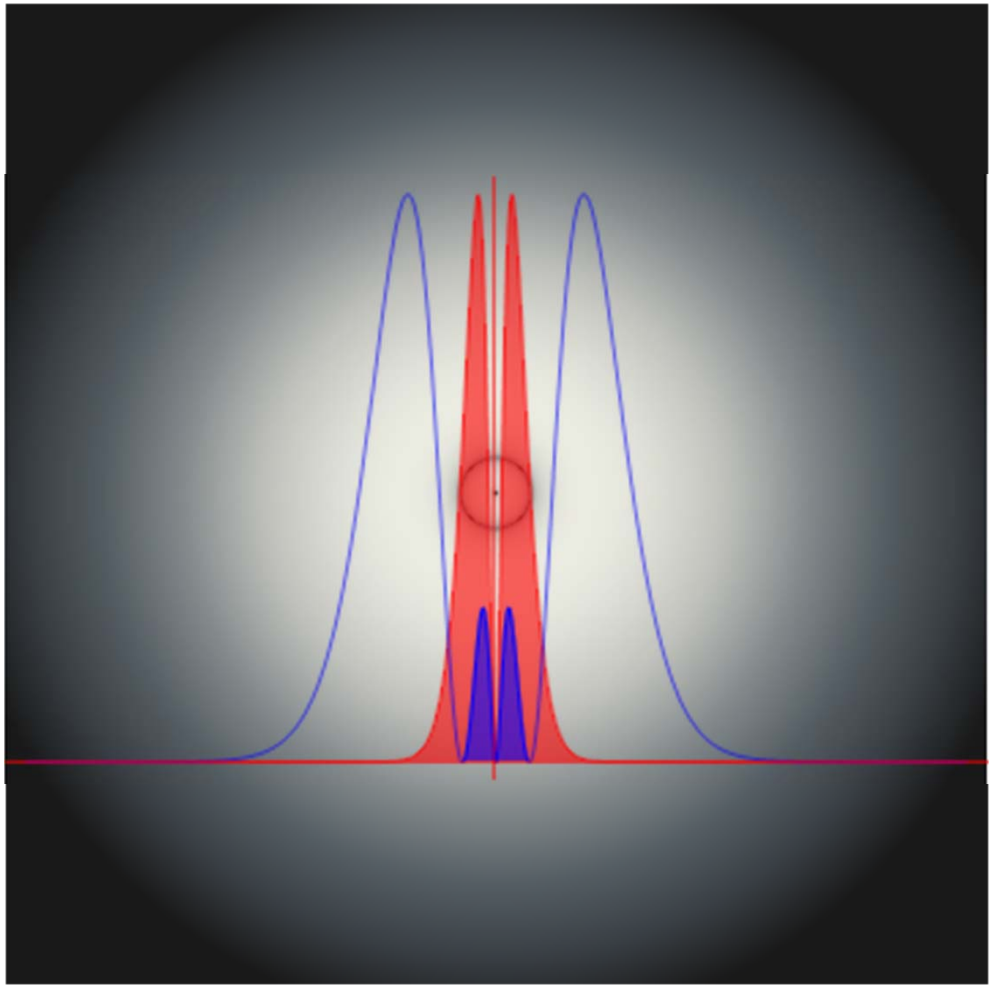
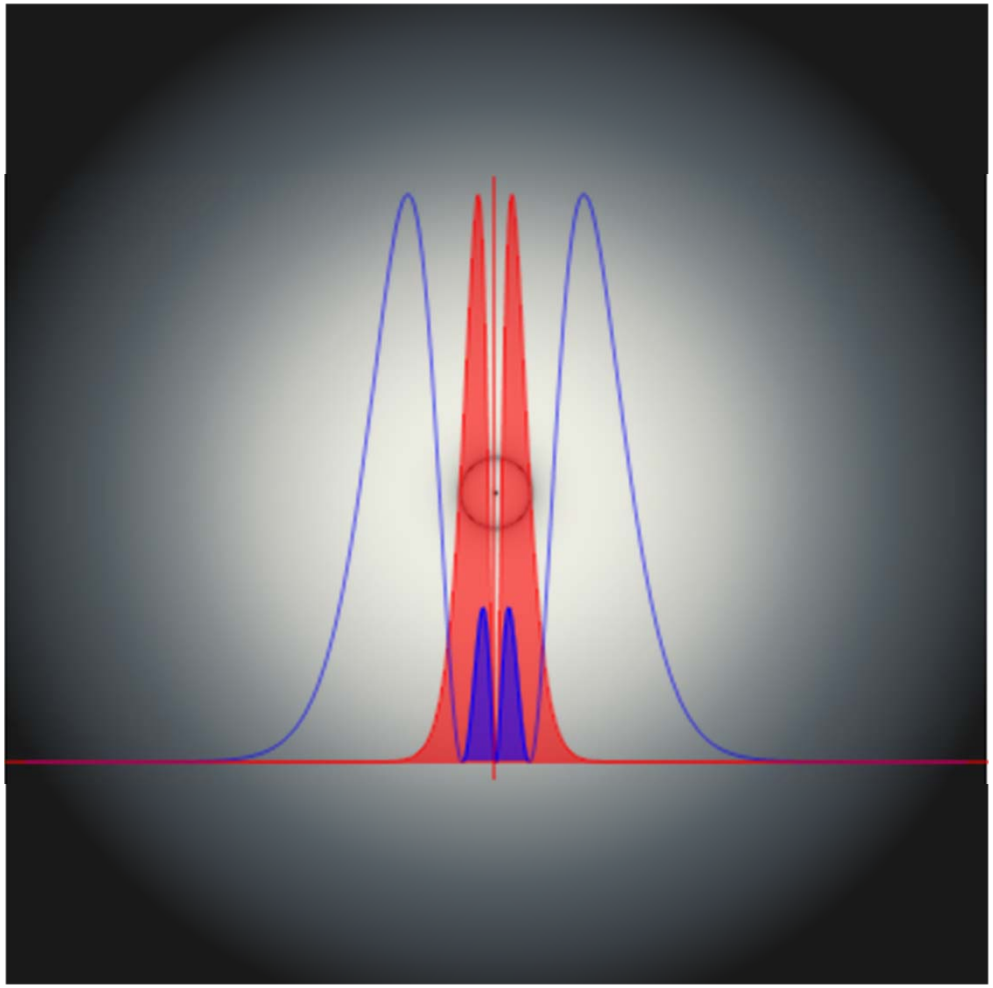
2s **inner loop** is **not shielded** by $1s^2$ cloud



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



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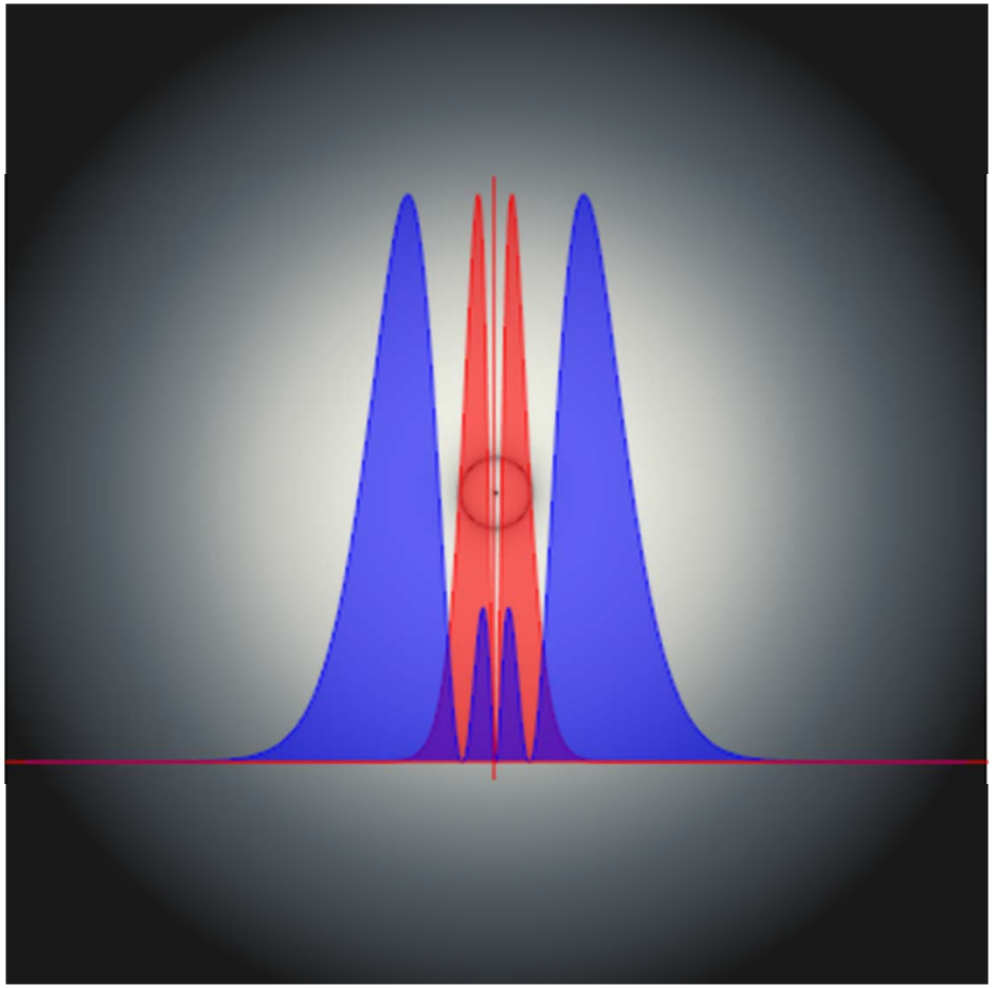
$$Z_{eff,2s} = Z_{eff,outer} + Z_{eff,inner} = 0.9 + 0.3 = 1.2$$

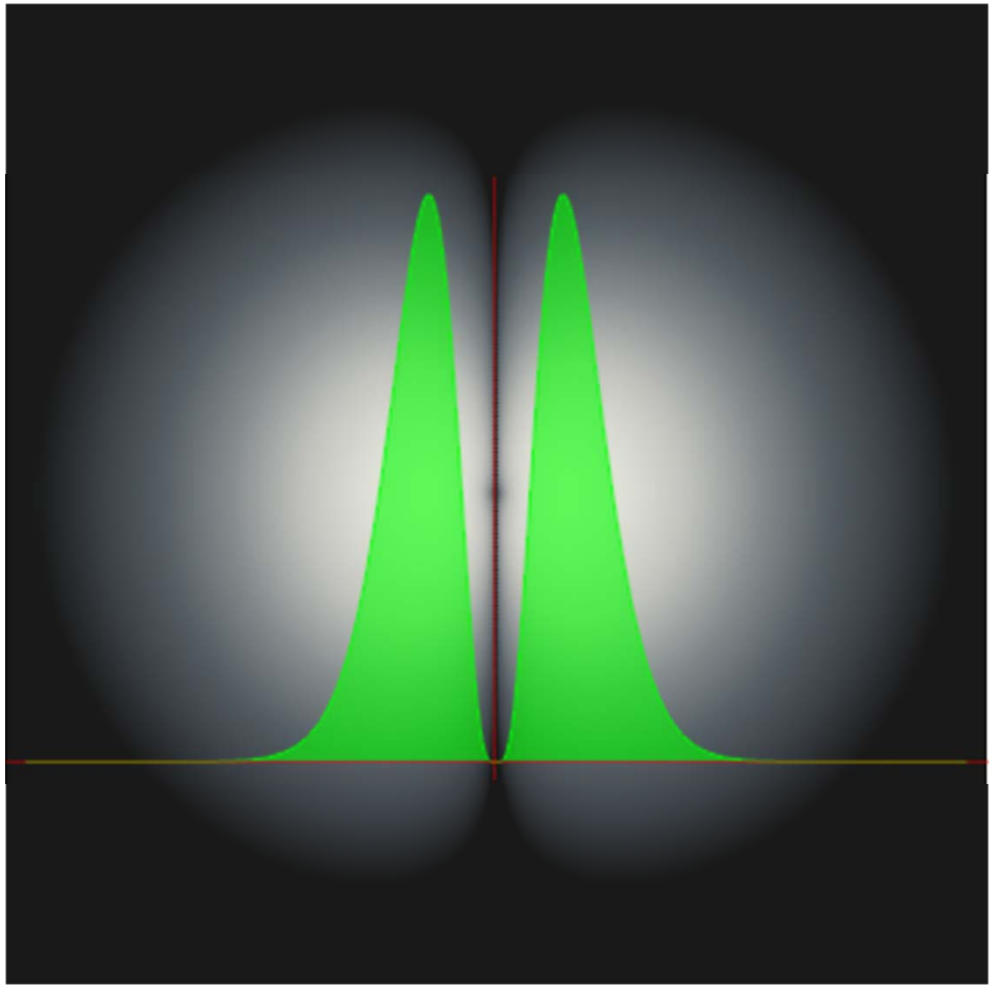


Li $1s^2 2s$ valence electron energy

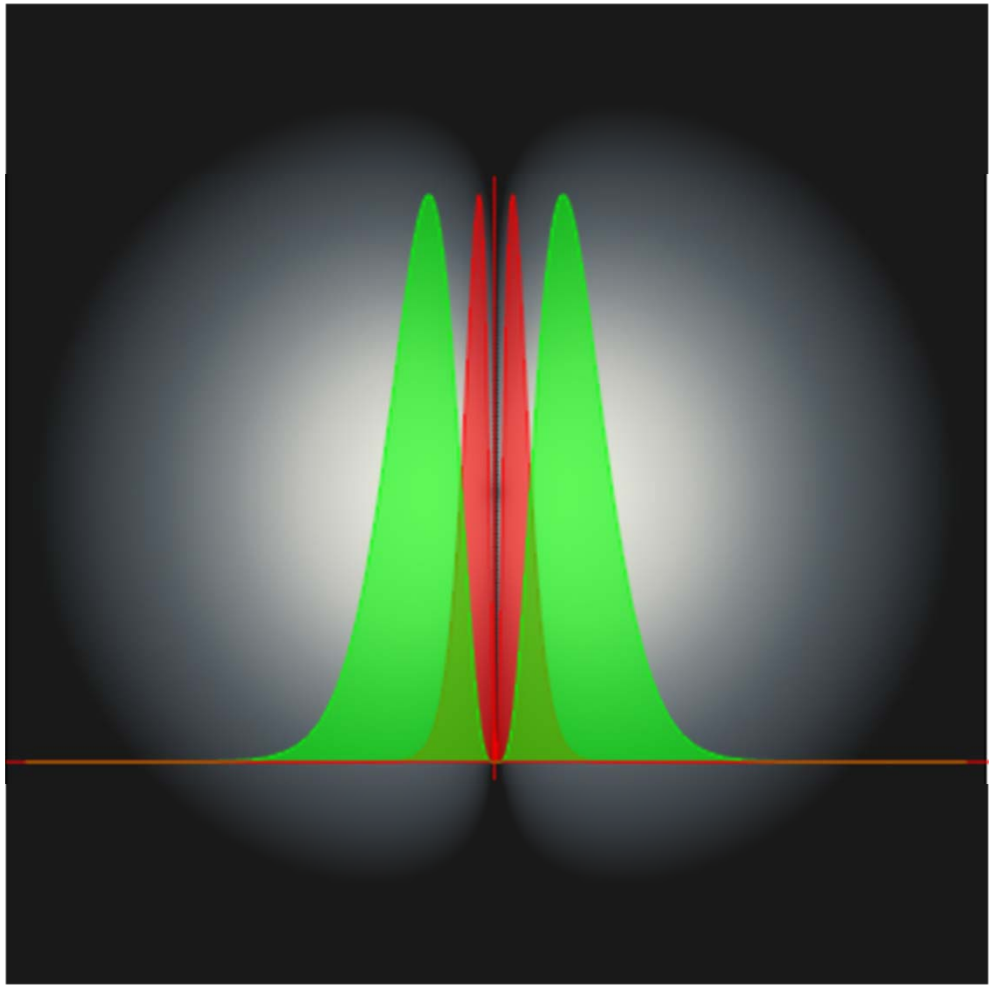
$$E_{2s} = -13.6 \text{ eV } \mathbf{Z_{eff,2s}^2}/4$$

$$= -13.6\text{eV} \times \mathbf{1.2^2}/4 = \mathbf{-4.90\ eV}$$

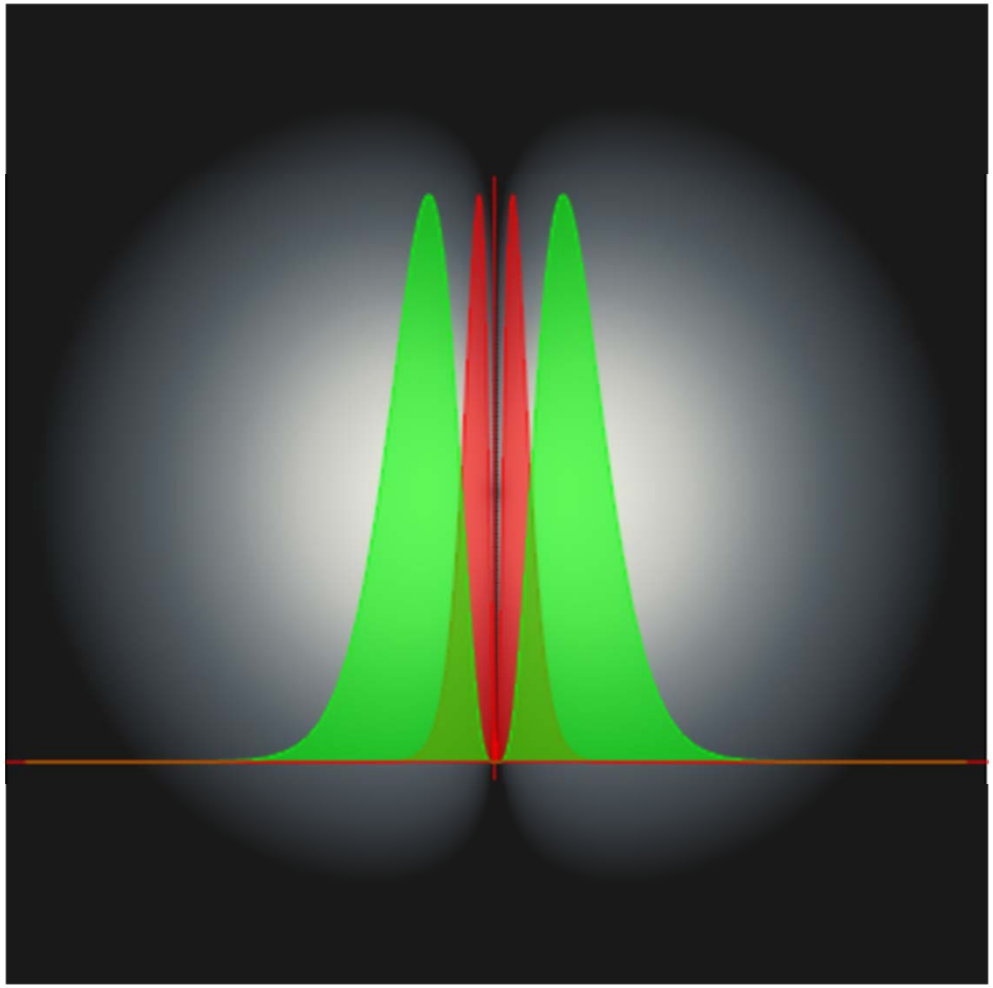
2p portion of Li $1s^2 2p$ electron cloud



2p **is shielded** by $1s^2$ cloud



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



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Li $1s^2 2p$ valence electron energy

$$E_{2p} = -13.6 \text{ eV } \mathbf{Z_{eff,2p}}^2/4$$

$$= -13.6 \text{ eV x } \mathbf{1^2}/4 = \mathbf{-3.40 \text{ eV}}$$

Li $1s^2 2s$ more stable than Li $1s^2 2p$

$$E_{2s} = -13.6 \text{ eV } \mathbf{Z_{eff,2s}^2}/4$$

$$= -13.6\text{eV x } \mathbf{1.2^2}/4 = \mathbf{-4.90\ eV}$$

$$E_{2p} = -13.6 \text{ eV } \mathbf{Z_{eff,2p}^2}/4$$

$$= -13.6 \text{ eV x } \mathbf{1^2}/4 = \mathbf{-3.40\ eV}$$